Philippe Derreumaux

List of Publications by Citations

164 papers	8,461 citations	54 h-index	86 g-index
169 ext. papers	9,733 ext. citations	5.4 avg, IF	6.53 L-index

#	Paper	IF	Citations
164	Amyloid -Protein and Alzheimer's Disease: When Computer Simulations Complement Experimental Studies. *Chemical Reviews*, **2015**, 115, 3518-63	68.1	426
163	PEP-FOLD: an updated de novo structure prediction server for both linear and disulfide bonded cyclic peptides. *Nucleic Acids Research*, **2012**, 40, W288-93	20.1	400
162	PEP-FOLD3: faster de novo structure prediction for linear peptides in solution and in complex. *Nucleic Acids Research*, **2016**, 44, W449-54	20.1	399
161	Improved PEP-FOLD Approach for Peptide and Miniprotein Structure Prediction. *Journal of Chemical Theory and Computation*, **2014**, 10, 4745-58	6.4	373
160	PEP-FOLD: an online resource for de novo peptide structure prediction. *Nucleic Acids Research*, **2009**, 37, W498-503	20.1	279
159	Inhibition of protein aggregation and amyloid formation by small molecules. *Current Opinion in Structural Biology*, **2015**, 30, 50-56	8.1	210
158	A coarse-grained protein force field for folding and structure prediction. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 394-408	4.2	160
157	Molecular mechanism of the inhibition of EGCG on the Alzheimer A(1-42) dimer. *Journal of Physical Chemistry B*, **2013**, 117, 3993-4002	3.4	149
156	Carbon nanotube inhibits the formation of -sheet-rich oligomers of the Alzheimer's amyloid-(16-22) peptide. *Biophysical Journal*, **2011**, 101, 2267-76	2.9	140
155	A fast method for large-scale de novo peptide and miniprotein structure prediction. *Journal of Computational Chemistry*, **2010**, 31, 726-38	3.5	140
154	Effects of all-atom force fields on amyloid oligomerization: replica exchange molecular dynamics simulations of the A(16-22) dimer and trimer. *Physical Chemistry Chemical Physics*, **2011**, 13, 9778-88	3.6	138
153	Why Is Research on Amyloid-Failing to Give New Drugs for Alzheimer's Disease?. *ACS Chemical Neuroscience*, **2017**, 8, 1435-1437	5.7	137
152	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. *Chemical Reviews*, **2021**, 121, 2545-2647	68.1	128
151	In silico assembly of Alzheimer's Abeta16-22 peptide into beta-sheets. *Journal of the American Chemical Society*, **2004**, 126, 11509-16	16.4	125
150	Pathway complexity of Alzheimer's beta-amyloid Abeta16-22 peptide assembly. *Structure*, **2004**, 12, 1245-55	5.5	121
149	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. *Chemical Society Reviews*, **2014**, 43, 4871-93	58.5	118
148	Thermodynamics and dynamics of amyloid peptide oligomerization are sequence dependent. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 954-63	4.2	102

147	Understanding amyloid fibril nucleation and a□oligomer/drug interactions from computer simulations. *Accounts of Chemical Research*, **2014**, 47, 603-11	24.3	100
146	High-Resolution Structures of the Amyloid-□1-42 Dimers from the Comparison of Four Atomistic Force Fields. *Journal of Physical Chemistry B*, **2017**, 121, 5977-5987	3.4	92
145	Structures of A□17-42 trimers in isolation and with five small-molecule drugs using a hierarchical computational procedure. *Journal of Physical Chemistry B*, **2012**, 116, 8412-22	3.4	92
144	Structures and thermodynamics of Alzheimer's amyloid-beta Abeta(16-35) monomer and dimer by replica exchange molecular dynamics simulations: implication for full-length Abeta fibrillation. *Journal of Physical Chemistry B*, **2009**, 113, 7668-75	3.4	92
143	Role of the region 23-28 in Abeta fibril formation: insights from simulations of the monomers and dimers of Alzheimer's peptides Abeta40 and Abeta42. *Current Alzheimer Research*, **2008**, 5, 244-50	3	91
142	From polypeptide sequences to structures using Monte Carlo simulations and an optimized potential. *Journal of Chemical Physics*, **1999**, 111, 2301-2310	3.9	91
141	Distinct dimerization for various alloforms of the amyloid-beta protein: A□(1-40), A□(1-42), and A□(1-40)(D23N). *Journal of Physical Chemistry B*, **2012**, 116, 4043-55	3.4	90
140	Coarse-grained protein molecular dynamics simulations. *Journal of Chemical Physics*, **2007**, 126, 025101	3.9	84
139	Structural and hydration properties of the partially unfolded states of the prion protein. *Biophysical Journal*, **2007**, 93, 1284-92	2.9	82
138	HiRE-RNA: a high resolution coarse-grained energy model for RNA. *Journal of Physical Chemistry B*, **2010**, 114, 11957-66	3.4	81
137	Exploring the early steps of amyloid peptide aggregation by computers. *Accounts of Chemical Research*, **2005**, 38, 885-91	24.3	81
136	The coarse-grained OPEP force field for non-amyloid and amyloid proteins. *Journal of Physical Chemistry B*, **2012**, 116, 8741-52	3.4	80
135	Impact of the mutation A21G (Flemish variant) on Alzheimer's beta-amyloid dimers by molecular dynamics simulations. *Biophysical Journal*, **2006**, 91, 3829-40	2.9	79
134	Effect of the Tottori familial disease mutation (D7N) on the monomers and dimers of A□40 and A□42. *ACS Chemical Neuroscience*, **2013**, 4, 1446-57	5.7	77
133	Induced beta-barrel formation of the Alzheimer's Abeta25-35 oligomers on carbon nanotube surfaces: implication for amyloid fibril inhibition. *Biophysical Journal*, **2009**, 97, 1795-803	2.9	76
132	Complex folding pathways in a simple beta-hairpin. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 464-74	4.2	76
131	The loop opening/closing motion of the enzyme triosephosphate isomerase. *Biophysical Journal*, **1998**, 74, 72-81	2.9	75
130	Distinct Morphologies for Amyloid Beta Protein Monomer: A□1-40, A□1-42, and A□1-40(D23N). *Journal of Chemical Theory and Computation*, **2011**, 7, 2584-92	6.4	71

129	Self-assembly of the beta2-microglobulin NHVTLSQ peptide using a coarse-grained protein model reveals a beta-barrel species. *Journal of Physical Chemistry B*, **2008**, 112, 4410-8	3.4	71
128	Sampling the self-assembly pathways of KFFE hexamers. *Biophysical Journal*, **2004**, 87, 3648-56	2.9	69
127	A multiscale approach to characterize the early aggregation steps of the amyloid-forming peptide GNNQQNY from the yeast prion sup-35. *PLoS Computational Biology*, **2011**, 7, e1002051	5	68
126	Replica exchange molecular dynamics simulations of coarse-grained proteins in implicit solvent. *Journal of Physical Chemistry B*, **2009**, 113, 267-74	3.4	67
125	Structures of the Alzheimer's Wild-Type Aβ1-40 Dimer from Atomistic Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 10478-87	3.4	66
124	Flexibility and binding affinity in protein-ligand, protein-protein and multi-component protein interactions: limitations of current computational approaches. *Journal of the Royal Society Interface* , **2012**, 9, 20-33	4.1	64
123	Targeting the early steps of Abeta16-22 protofibril disassembly by N-methylated inhibitors: a numerical study. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 442-52	4.2	63
122	Coarse-grained simulations of RNA and DNA duplexes. *Journal of Physical Chemistry B*, **2013**, 117, 8047-60	3.4	60
121	The conformations of the amyloid-beta (21-30) fragment can be described by three families in solution. *Journal of Chemical Physics*, **2006**, 125, 084911	3.9	60
120	Atomic and dynamic insights into the beneficial effect of the 1,4-naphthoquinon-2-yl-L-tryptophan inhibitor on Alzheimer's Aβ1-42 dimer in terms of aggregation and toxicity. *ACS Chemical Neuroscience*, **2014**, 5, 148-59	5.7	59
119	Computational simulations of the early steps of protein aggregation. *Prion*, **2007**, 1, 3-8	2.3	59
118	Low molecular weight oligomers of amyloid peptides display beta-barrel conformations: a replica exchange molecular dynamics study in explicit solvent. *Journal of Chemical Physics*, **2010**, 132, 165103	3.9	58
117	Following the aggregation of amyloid-forming peptides by computer simulations. *Journal of Chemical Physics*, **2005**, 122, 174904	3.9	57
116	The antitumor properties of the alpha3(IV)-(185-203) peptide from the NC1 domain of type IV collagen (tumstatin) are conformation-dependent. *Journal of Biological Chemistry*, **2004**, 279, 2091-100	5.4	57
115	Familial Alzheimer A2 V mutation reduces the intrinsic disorder and completely changes the free energy landscape of the Aβ1-28 monomer. *Journal of Physical Chemistry B*, **2014**, 118, 501-10	3.4	56
114	Generating ensemble averages for small proteins from extended conformations by Monte Carlo simulations. *Physical Review Letters*, **2000**, 85, 206-9	7.4	56
113	A new spectroscopic molecular mechanics force field. Parameters for proteins. *Journal of Chemical Physics*, **1995**, 102, 8586-8605	3.9	56
112	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of AβDimer. *Journal of Chemical Theory and Computation*, **2019**, 15, 1440-1452	6.4	55

111	Sampling the complex energy landscape of a simple β-hairpin. *Journal of Chemical Physics*, **2003**, 119, 6403-6406	3.9	54
110	Epock: rapid analysis of protein pocket dynamics. *Bioinformatics*, **2015**, 31, 1478-80	7.2	53
109	Structures of soluble amyloid oligomers from computer simulations. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 180-91	4.2	52
108	Structures of the intrinsically disordered Aβ, tau and α-synuclein proteins in aqueous solution from computer simulations. *Biophysical Chemistry*, **2020**, 264, 106421	3.5	49
107	A truncated Newton minimizer adapted for CHARMM and biomolecular applications. *Journal of Computational Chemistry*, **1994**, 15, 532-552	3.5	48
106	Protein Simulations in Fluids: Coupling the OPEP Coarse-Grained Force Field with Hydrodynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 1843-53	6.4	46
105	Exploring the energy landscape of proteins: A characterization of the activation-relaxation technique. *Journal of Chemical Physics*, **2002**, 117, 11379-11387	3.9	46
104	Computer simulations aimed at structure prediction of supersecondary motifs in proteins. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 159-66	4.2	45
103	The structures and vibrational frequencies of a series of alkanes using the SPASIBA force field. *Journal of Molecular Structure*, **1993**, 295, 203-221	3.4	44
102	A diffusion process-controlled Monte Carlo method for finding the global energy minimum of a polypeptide chain. I. Formulation and test on a hexadecapeptide. *Journal of Chemical Physics*, **1997**, 106, 5260-5270	3.9	42
101	Impact of the A2V Mutation on the Heterozygous and Homozygous Aβ1-40 Dimer Structures from Atomistic Simulations. *ACS Chemical Neuroscience*, **2016**, 7, 823-32	5.7	42
100	Effect of the English familial disease mutation (H6R) on the monomers and dimers of Aβ40 and Aβ42. *ACS Chemical Neuroscience*, **2014**, 5, 646-57	5.7	41
99	Communication: Simulated tempering with fast on-the-fly weight determination. *Journal of Chemical Physics*, **2013**, 138, 061102	3.9	39
98	Structural diversity of the soluble trimers of the human amylin(20-29) peptide revealed by molecular dynamics simulations. *Journal of Chemical Physics*, **2009**, 130, 125101	3.9	39
97	Folding a 20 amino acid β-peptide with the diffusion process-controlled Monte Carlo method. *Journal of Chemical Physics*, **1997**, 107, 1941-1947	3.9	39
96	A vibrational molecular force field of model compounds with biological interest. I. Harmonic dynamics of crystalline urea at 123 K. *Journal of Computational Chemistry*, **1990**, 11, 560-568	3.5	39
95	The conversion of helix H2 to beta-sheet is accelerated in the monomer and dimer of the prion protein upon T183A mutation. *Journal of Physical Chemistry B*, **2009**, 113, 6942-8	3.4	38
94	Hydrodynamic effects on β-amyloid (16-22) peptide aggregation. *Journal of Chemical Physics*, **2016**, 145, 035102	3.9	37

93	Self-assembly of amyloid-forming peptides by molecular dynamics simulations. *Frontiers in Bioscience - Landmark*, **2008**, 13, 5681-92	2.8	37
92	Coarse-Grained HiRE-RNA Model for ab Initio RNA Folding beyond Simple Molecules, Including Noncanonical and Multiple Base Pairings. *Journal of Chemical Theory and Computation*, **2015**, 11, 3510-22	6.4	35
91	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. *Journal of Chemical Theory and Computation*, **2016**, 12, 6077-6097	6.4	35
90	Importance of the ion-pair interactions in the OPEP coarse-grained force field: parametrization and validation. *Journal of Chemical Theory and Computation*, **2013**, 9, 4574-4584	6.4	35
89	Impact of the tail and mutations G131V and M129V on prion protein flexibility. *Proteins: Structure, Function and Bioinformatics*, **2003**, 51, 258-65	4.2	35
88	Folding Atomistic Proteins in Explicit Solvent Using Simulated Tempering. *Journal of Physical Chemistry B*, **2015**, 119, 6941-51	3.4	34
87	Conformational studies of neuroactive ligands. 1. Force field and vibrational spectra of crystalline acetylcholine. *The Journal of Physical Chemistry*, **1989**, 93, 1338-1350		33
86	Dimerization Mechanism of Alzheimer A□Peptides: The High Content of Intrapeptide-Stabilized Conformations in A2V and A2T Heterozygous Dimers Retards Amyloid Fibril Formation. *Journal of Physical Chemistry B*, **2016**, 120, 12111-12126	3.4	31
85	Evidence that the 127-164 region of prion proteins has two equi-energetic conformations with beta or alpha features. *Biophysical Journal*, **2001**, 81, 1657-65	2.9	31
84	Tetrameric A□40 and A□42 □Barrel Structures by Extensive Atomistic Simulations. I. In a Bilayer Mimicking a Neuronal Membrane. *Journal of Physical Chemistry B*, **2019**, 123, 3643-3648	3.4	30
83	Picosecond dissociation of amyloid fibrils with infrared laser: A nonequilibrium simulation study. *Journal of Chemical Physics*, **2015**, 143, 155101	3.9	30
82	Force-field and vibrational spectra of oligosaccharides with different glycosidic linkages□Part I. Trehalose dihydrate, sophorose monohydrate and laminaribiose. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1994**, 50, 87-104		30
81	Effects of G33A and G33I mutations on the structures of monomer and dimer of the amyloid-□ fragment 29-42 by replica exchange molecular dynamics simulations. *Journal of Physical Chemistry B*, **2011**, 115, 1282-8	3.4	29
80	Probing amyloid fibril formation of the NFGAIL peptide by computer simulations. *Journal of Chemical Physics*, **2007**, 126, 065101	3.9	29
79	Molecular structure of the NQTrp inhibitor with the Alzheimer A□1-28 monomer. *European Journal of Medicinal Chemistry*, **2015**, 91, 43-50	6.8	28
78	Improved greedy algorithm for protein structure reconstruction. *Journal of Computational Chemistry*, **2005**, 26, 506-13	3.5	27
77	Conformational Ensembles of the Wild-Type and S8C A□1-42 Dimers. *Journal of Physical Chemistry B*, **2017**, 121, 2434-2442	3.4	26
76	Conformational ensemble and polymorphism of the all-atom Alzheimer's A□(37-42) amyloid peptide oligomers. *Journal of Physical Chemistry B*, **2013**, 117, 5831-40	3.4	26

75	Substitutions at residue 211 in the prion protein drive a switch between CJD and GSS syndrome, a new mechanism governing inherited neurodegenerative disorders. *Human Molecular Genetics*, **2012**, 21, 5417-28	5.6	26
74	Intrinsic determinants of A(12-24) pH-dependent self-assembly revealed by combined computational and experimental studies. *PLoS ONE*, **2011**, 6, e24329	3.7	25
73	Assessing the Quality of the OPEP Coarse-Grained Force Field. *Journal of Chemical Theory and Computation*, **2011**, 7, 1928-34	6.4	25
72	Sampling activated mechanisms in proteins with the activation-relaxation technique. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 78-86	2.8	25
71	Electrostatics analysis of the mutational and pH effects of the N-terminal domain self-association of the major ampullate spidroin. *Soft Matter*, **2016**, 12, 5600-12	3.6	24
70	Energy landscapes of the monomer and dimer of the Alzheimer's peptide Abeta(1-28). *Journal of Chemical Physics*, **2008**, 128, 125108	3.9	24
69	Long timestep dynamics of peptides by the dynamics driver approach. *Proteins: Structure, Function and Bioinformatics*, **1995**, 21, 282-302	4.2	22
68	Tau R3-R4 Domain Dimer of the Wild Type and Phosphorylated Ser356 Sequences. I. In Solution by Atomistic Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 2975-2983	3.4	21
67	Tetrameric A40 and A42 Barrel Structures by Extensive Atomistic Simulations. II. In Aqueous Solution. *Journal of Physical Chemistry B*, **2019**, 123, 6750-6756	3.4	21
66	Amyloid oligomer structure characterization from simulations: a general method. *Journal of Chemical Physics*, **2014**, 140, 094105	3.9	21
65	Aggregating the amyloid Abeta(11-25) peptide into a four-stranded beta-sheet structure. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 877-88	4.2	21
64	Coarse-grained and All-atom Simulations towards the Early and Late Steps of Amyloid Fibril Formation. *Israel Journal of Chemistry*, **2017**, 57, 564-573	3.4	20
63	Impact of Thermostats on Folding and Aggregation Properties of Peptides Using the Optimized Potential for Efficient Structure Prediction Coarse-Grained Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 1502-10	6.4	20
62	Dependency between consecutive local conformations helps assemble protein structures from secondary structures using Go potential and greedy algorithm. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 732-40	4.2	20
61	Nonequilibrium all-atom molecular dynamics simulation of the bubble cavitation and application to dissociate amyloid fibrils. *Journal of Chemical Physics*, **2016**, 145, 174113	3.9	20
60	Multiscale Aggregation of the Amyloid A Peptide: From Disordered Coagulation and Lateral Branching to Amorphous Prefibrils. *Journal of Physical Chemistry Letters*, **2019**, 10, 1594-1599	6.4	19
59	Probable Transmembrane Amyloid Helix Bundles Capable of Conducting Ca Ions. *Journal of Physical Chemistry B*, **2019**, 123, 2645-2653	3.4	19
58	Multi-scale simulations of biological systems using the OPEP coarse-grained model. *Biochemical and Biophysical Research Communications*, **2018**, 498, 296-304	3.4	19

57	Evaluation of the coarse-grained OPEP force field for protein-protein docking. *BMC Biophysics*, **2016**, 9, 4	0	19
56	Lattice model for amyloid peptides: OPEP force field parametrization and applications to the nucleus size of Alzheimer's peptides. *Journal of Chemical Physics*, **2016**, 144, 205103	3.9	19
55	Multiscale simulation of molecular processes in cellular environments. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2016**, 374,	3	19
54	Rayleigh-Plesset equation of the bubble stable cavitation in water: A nonequilibrium all-atom molecular dynamics simulation study. *Journal of Chemical Physics*, **2018**, 148, 094505	3.9	18
53	Combined experimental and simulation studies suggest a revised mode of action of the anti-Alzheimer disease drug NQ-Trp. *Chemistry - A European Journal*, **2015**, 21, 12657-66	4.8	18
52	Structural, thermodynamical, and dynamical properties of oligomers formed by the amyloid NNQQ peptide: insights from coarse-grained simulations. *Journal of Chemical Physics*, **2012**, 137, 025101	3.9	18
51	Molecular Mechanism of Protein Unfolding under Shear: A Lattice Boltzmann Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2018**, 122, 1573-1579	3.4	17
50	Protein-RNA complexation driven by the charge regulation mechanism. *Biochemical and Biophysical Research Communications*, **2018**, 498, 264-273	3.4	17
49	Structure and aggregation mechanism of beta(2)-microglobulin (83-99) peptides studied by molecular dynamics simulations. *Biophysical Journal*, **2007**, 93, 3353-62	2.9	17
48	Molecular Mechanism of the Cell Membrane Pore Formation Induced by Bubble Stable Cavitation. *Journal of Physical Chemistry B*, **2019**, 123, 71-78	3.4	17
47	Are coarse-grained models apt to detect protein thermal stability? The case of OPEP force field. *Journal of Non-Crystalline Solids*, **2015**, 407, 494-501	3.9	16
46	The complex folding pathways of protein A suggest a multiple-funnelled energy landscape. *Journal of Chemical Physics*, **2008**, 128, 045101	3.9	16
45	OPEP6: A New Constant-pH Molecular Dynamics Simulation Scheme with OPEP Coarse-Grained Force Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 3875-3888	6.4	15
44	VLITL is a major cross-β sheet signal for fibrinogen Aα chain frameshift variants. *Blood*, **2017**, 130, 2799-2807	12	15
43	Three Weaknesses for Three Perturbations: Comparing Protein Unfolding Under Shear, Force, and Thermal Stresses. *Journal of Physical Chemistry B*, **2018**, 122, 11922-11930	3.4	15
42	Probing the quality control mechanism of the twin-arginine translocase with folding variants of a -designed heme protein. *Journal of Biological Chemistry*, **2018**, 293, 6672-6681	5.4	14
41	Aggregation of disease-related peptides. *Progress in Molecular Biology and Translational Science*, **2020**, 170, 435-460	4	14
40	Influence of electric field on the amyloid-(29-42) peptides embedded in a membrane bilayer. *Journal of Chemical Physics*, **2018**, 148, 045105	3.9	13

39	Small static electric field strength promotes aggregation-prone structures in amyloid-β(29-42). *Journal of Chemical Physics*, **2017**, 146, 145101	3.9	12
38	Picosecond melting of peptide nanotubes using an infrared laser: a nonequilibrium simulation study. *Physical Chemistry Chemical Physics*, **2015**, 17, 27275-80	3.6	12
37	Stability of Aβ11-40 Trimers with Parallel and Antiparallel β-Sheet Organizations in a Membrane-Mimicking Environment by Replica Exchange Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2020**, 124, 617-626	3.4	12
36	Ab initio RNA folding. *Journal of Physics Condensed Matter*, **2015**, 27, 233102	1.8	12
35	Exploring energy landscapes of protein folding and aggregation. *Frontiers in Bioscience - Landmark*, **2008**, 13, 4495-516	2.8	12
34	Fast coarse-grained model for RNA titration. *Journal of Chemical Physics*, **2017**, 146, 035101	3.9	11
33	Impact of A2T and D23N Mutations on Tetrameric Aβ42 Barrel within a Dipalmitoylphosphatidylcholine Lipid Bilayer Membrane by Replica Exchange Molecular Dynamics. *Journal of Physical Chemistry B*, **2020**, 124, 1175-1182	3.4	11
32	Amyloid-β(29-42) Dimeric Conformations in Membranes Rich in Omega-3 and Omega-6 Polyunsaturated Fatty Acids. *Journal of Physical Chemistry B*, **2019**, 123, 2687-2696	3.4	11
31	Modelling lipid systems in fluid with Lattice Boltzmann Molecular Dynamics simulations and hydrodynamics. *Scientific Reports*, **2019**, 9, 16450	4.9	11
30	Adequate prediction for inhibitor affinity of Aβ protofibril using the linear interaction energy method.. *RSC Advances*, **2019**, 9, 12455-12461	3.7	10
29	Infrared Laser-Induced Amyloid Fibril Dissociation: A Joint Experimental/Theoretical Study on the GNNQQNY Peptide. *Journal of Physical Chemistry B*, **2020**, 124, 6266-6277	3.4	10
28	Impact of the Astaxanthin, Betanin, and EGCG Compounds on Small Oligomers of Amyloid Aβ Peptide. *Journal of Chemical Information and Modeling*, **2020**, 60, 1399-1408	6.1	10
27	Exploring the early steps of aggregation of amyloid-forming peptide KFFE. *Journal of Physics Condensed Matter*, **2004**, 16, S5047-S5054	1.8	10
26	Insight into protein topology from Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 117, 3499-3503	3.9	10
25	Communication: Multiple atomistic force fields in a single enhanced sampling simulation. *Journal of Chemical Physics*, **2015**, 143, 021101	3.9	9
24	Interaction mechanism between the focused ultrasound and lipid membrane at the molecular level. *Journal of Chemical Physics*, **2019**, 150, 215101	3.9	7
23	Picosecond infrared laser-induced all-atom nonequilibrium molecular dynamics simulation of dissociation of viruses. *Physical Chemistry Chemical Physics*, **2016**, 18, 11951-8	3.6	7
22	Replica-exchange molecular dynamics simulation for understanding the initial process of amyloid peptide aggregation. *Molecular Simulation*, **2015**, 41, 1041-1044	2	7

21	C-Terminal Plays as the Possible Nucleation of the Self-Aggregation of the S-Shape A Tetramer in Solution: Intensive MD Study. *ACS Omega*, **2019**, 4, 11066-11073	3.9	6
20	Coarse-grained models for protein folding and aggregation. *Methods in Molecular Biology*, **2013**, 924, 585-600	1.4	6
19	In silico structural characterization of protein targets for drug development against Trypanosoma cruzi. *Journal of Molecular Modeling*, **2016**, 22, 244	2	6
18	Breaking down cellulose fibrils with a mid-infrared laser. *Cellulose*, **2018**, 25, 5553-5568	5.5	5
17	The betaalphabetaalphabeta elementary supersecondary structure of the Rossmann fold from porcine lactate dehydrogenase exhibits characteristics of a molten globule. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 740-5	4.2	5
16	Molecular mechanism of ultrasound interaction with a blood brain barrier model. *Journal of Chemical Physics*, **2020**, 153, 045104	3.9	5
15	Cholesterol Molecules Alter the Energy Landscape of Small A 1-42 Oligomers. *Journal of Physical Chemistry B*, **2021**, 125, 2299-2307	3.4	5
14	What Can Human-Guided Simulations Bring to RNA Folding?. *Biophysical Journal*, **2017**, 113, 302-312	2.9	4
13	Amyloid- Drug Interactions from Computer Simulations and Cell-Based Assays. *Journal of Alzheimer's Disease*, **2018**, 64, S659-S672	4.3	4
12	A Computational Methodology to Overcome the Challenges Associated With the Search for Specific Enzyme Targets to Develop Drugs Against. *Bioinformatics and Biology Insights*, **2017**, 11, 1177932217712471	5.3	3
11	Effects of the RGTFEGKF inhibitor on the structures of the transmembrane fragment 70-86 of glycophorin A: an all-atom molecular dynamics study. *Journal of Physical Chemistry B*, **2010**, 114, 1004-9	3.4	3
10	Exposure of Von Willebrand Factor Cleavage Site in A1A2A3-Fragment under Extreme Hydrodynamic Shear. *Polymers*, **2021**, 13,	4.5	3
9	Nonequilibrium atomistic molecular dynamics simulation of tubular nanomotor propelled by bubble propulsion. *Journal of Chemical Physics*, **2019**, 151, 024103	3.9	2
8	Mesoscale biosimulations within a unified framework: from proteins to plasmids. *Molecular Simulation*, **2021**, 47, 101-112	2	2
7	Nonequilibrium molecular dynamics simulations of infrared laser-induced dissociation of a tetrameric A 42 barrel in a neuronal membrane model. *Chemistry and Physics of Lipids*, **2021**, 234, 105030	3.7	2
6	Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. *Langmuir*, **2021**, 37, 7945-7954	4	1
5	Computer Simulations Aimed at Exploring Protein Aggregation and Dissociation.. *Methods in Molecular Biology*, **2022**, 2340, 175-196	1.4	1
4	Impact of the Rat R5G, Y10F, and H13R Mutations on Tetrameric A 42 Barrel in a Lipid Bilayer Membrane Model. *Journal of Physical Chemistry B*, **2021**, 125, 3105-3113	3.4	0

List of Publications

3 Exploring the Structures of β-Amyloid Oligomers in Aqueous Solution Using Coarse-Grained Protein Models. *Modecular Medicine and Medicinal*, **2013**, 283-303

2 Exploring amyloid aggregates with coarse-grained protein simulations. *Materials Research Society Symposia Proceedings*, **2013**, 1535, 6001

1 Dynamics of Amyloid Formation from Simplified Representation to Atomistic Simulations.. *Methods in Molecular Biology*, **2022**, 2405, 95-113 1.4