Dmitri K Klimov

List of Publications by Year
in descending order

53	2,074	304743	233421
papers	citations	22 h-index	45 g-index

53	53	53	1802
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Protein folding kinetics: timescales, pathways and energy landscapes in terms of sequence-dependent properties. Folding & Design, 1997, 2, 1-22.	4.5	390
2	Dissecting the Assembly of AÎ²16â€“22 Amyloid Peptides into Antiparallel Î² Sheets. Structure, 2003, 11, 295-307.	3.3	360
3	Aqueous urea solution destabilizes AÂ16-22 oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 14760-14765.	7.1	151
4	Interpeptide interactions induce helix to strand structural transition in AÎ² peptides. Proteins: Structure, Function and Bioinformatics, 2009, 77, 1-13.	2.6	141
5	Replica Exchange Simulations of the Thermodynamics of AÎ² Fibril Growth. Biophysical Journal, 2009, 96, 442-452.	0.5	95
6	Molecular Dynamics Simulations of Ibuprofen Binding to AÎ² Peptides. Biophysical Journal, 2009, 97, 2070-2079.	0.5	53
7	Symmetric Connectivity of Secondary Structure Elements Enhances the Diversity of Folding Pathways. Journal of Molecular Biology, 2005, 353, 1171-1186.	4.2	50
8	Probing Energetics of AÎ² Fibril Elongation by Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 4428-4437.	0.5	49
9	Multiple stepwise refolding of immunoglobulin domain I27 upon force quench depends on initial conditions. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 93-98.	7.1	47
10	Does Replica Exchange with Solute Tempering Efficiently Sample AÎ² Peptide Conformational Ensembles?. Journal of Chemical Theory and Computation, 2016, 12, 5201-5214.	5.3	47
11	Alzheimerâ€™s AÎ²10â€“40 Peptide Binds and Penetrates DMPC Bilayer: An Isobaricâ€“Isothermal Replica Exchange Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 2638-2648.	2.6	45
12	Mapping Conformational Ensembles of AÎ² Oligomers in Molecular Dynamics Simulations. Biophysical Journal, 2010, 99, 1949-1958.	0.5	41
13	Probing the Effect of Amino-Terminal Truncation for AÎ²1â^'40 Peptides. Journal of Physical Chemistry B, 2009, 113, 6692-6702.	2.6	40
14	Explicit Solvent Molecular Dynamics Simulations of AÎ² Peptide Interacting with Ibuprofen Ligands. Journal of Physical Chemistry B, 2012, 116, 12922-12932.	2.6	33
15	Binding of nonsteroidal antiâ€inflammatory drugs to AÎ² fibril. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2849-2860.	2.6	30
16	Dissociation of AÎ²16â€“22 Amyloid Fibrils Probed by Molecular Dynamics. Journal of Molecular Biology, 2007, 368, 1202-1213.	4.2	28
17	Binding of Cytotoxic AÎ²25â€“35 Peptide to the Dimyristoylphosphatidylcholine Lipid Bilayer. Journal of Chemical Information and Modeling, 2018, 58, 1053-1065.	5.4	28
18	Molecular Dynamics Simulations of Anti-Aggregation Effect of Ibuprofen. Biophysical Journal, 2010, 98, 2662-2670.	0.5	26

#	Article	IF	Citations
19	Nonsteroidal Anti-inflammatory Drug Naproxen Destabilizes AÎ² Amyloid Fibrils: A Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2010, 114, 15394-15402.	2.6	24
20	Side Chain Interactions Can Impede Amyloid Fibril Growth: Replica Exchange Simulations of AÎ² Peptide Mutant. Journal of Physical Chemistry B, 2009, 113, 11848-11857.	2.6	23
21	Naproxen Interferes with the Assembly of AÎ² Oligomers Implicated in Alzheimer's Disease. Biophysical Journal, 2011, 100, 2024-2032.	0.5	23
22	Binding of AÎ² peptide creates lipid density depression in DMPC bilayer. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2678-2688.	2.6	22
23	Cholesterol Changes the Mechanisms of AÎ² Peptide Binding to the DMPC Bilayer. Journal of Chemical Information and Modeling, 2017, 57, 2554-2565.	5.4	22
24	Is the Conformational Ensemble of Alzheimerâ€™s AÎ²10-40 Peptide Force Field Dependent?. PLoS Computational Biology, 2017, 13, e1005314.	3.2	22
25	Temperature-Induced Dissociation of AÎ² Monomers from Amyloid Fibril. Biophysical Journal, 2008, 95, 1758-1772.	0.5	21
26	De novo aggregation of Alzheimerâ€™s AÎ²25-35 peptides in a lipid bilayer. Scientific Reports, 2019, 9, 7161.	3.3	21
27	Lattice simulations of cotranslational folding of single domain proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 925-937.	2.6	18
28	Calcium Enhances Binding of A Î² Monomer to DMPC Lipid Bilayer. Biophysical Journal, 2015, 108, 1807-1818.	0.5	16
29	Mechanical Unbinding of AÎ² Peptides from Amyloid Fibrils. Journal of Molecular Biology, 2007, 373, 785-800.	4.2	15
30	Molecular Interactions of Alzheimer's Biomarker FDDNP with AÎ² Peptide. Biophysical Journal, 2012, 103, 2341-2351.	0.5	15
31	The Alzheimer's disease A Î² peptide binds to the anionic DMPS lipid bilayer. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1118-1128.	2.6	15
32	Predicting Genetic Variation Severity Using Machine Learning to Interpret Molecular Simulations. Biophysical Journal, 2021, 120, 189-204.	0.5	15
33	Molecular Mechanisms of Alzheimerâ€™s Biomarker FDDNP Binding to AÎ² Amyloid Fibril. Journal of Physical Chemistry B, 2015, 119, 11568-11580.	2.6	14
34	Methionine Oxidation Changes the Mechanism of AÎ² Peptide Binding to the DMPC Bilayer. Scientific Reports, 2019, 9, 5947.	3.3	13
35	Computational Backbone Mutagenesis of AÎ² Peptides: Probing the Role of Backbone Hydrogen Bonds in Aggregation. Journal of Physical Chemistry B, 2010, 114, 4755-4762.	2.6	12
36	Molecular Dynamics Investigation of the Ternary Bilayer Formed by Saturated Phosphotidylcholine, Sphingomyelin, and Cholesterol. Journal of Physical Chemistry B, 2018, 122, 11311-11325.	2.6	11

#	Article	IF	Citations
37	Three Popular Force Fields Predict Consensus Mechanism of Amyloid Î² Peptide Binding to the Dimyristoylgylcerophosphocholine Bilayer. Journal of Chemical Information and Modeling, 2020, 60, 2282-2293.	5.4	11
38	Binding to the lipid monolayer induces conformational transition in AÎ² monomer. Journal of Molecular Modeling, 2013, 19, 737-750.	1.8	9
39	Folding of tandem-linked domains. Proteins: Structure, Function and Bioinformatics, 2007, 67, 795-810.	2.6	8
40	Phosphorylation Promotes AÎ²25â€“35 Peptide Aggregation within the DMPC Bilayer. ACS Chemical Neuroscience, 2020, 11, 3430-3441.	3.5	8
41	Machine learning-based prediction of drug and ligand binding in BCL-2 variants through molecular dynamics. Computers in Biology and Medicine, 2022, 140, 105060.	7.0	8
42	Globular state in the oligomers formed by AÎ² peptides. Journal of Chemical Physics, 2010, 132, 225101.	3.0	7
43	Revealing Hidden Helix Propensity in AÎ² Peptides by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 12030-12038.	2.6	7
44	Do Cholesterol and Sphingomyelin Change the Mechanism of AÎ²_{25â€“35} Peptide Binding to Zwitterionic Bilayer?. Journal of Chemical Information and Modeling, 2019, 59, 5207-5217.	5.4	7
45	Met35 Oxidation Hinders AÎ²25-35 Peptide Aggregation within the Dimyristoylphosphatidylcholine Bilayer. ACS Chemical Neuroscience, 2021, 12, 3225-3236.	3.5	7
46	Inclusion of lipopeptides into the DMPC lipid bilayers prevents AÎ² peptide insertion. Physical Chemistry Chemical Physics, 2017, 19, 10087-10098.	2.8	6
47	Mechanisms of Binding of Antimicrobial Peptide PGLa to DMPC/DMPG Membrane. Journal of Chemical Information and Modeling, 2022, 62, 1525-1537.	5.4	5
48	Partitioning of Benzoic Acid into 1,2-Dimyristoyl-sn-glycero-3-phosphocholine and Bloodâ€“Brain Barrier Mimetic Bilayers. Journal of Chemical Information and Modeling, 2020, 60, 4030-4046.	5.4	4
49	Does amino acid sequence determine the properties of AÎ² dimer?. Journal of Chemical Physics, 2011, 135, 035103.	3.0	3
50	Greedy replica exchange algorithm for heterogeneous computing grids. Journal of Molecular Modeling, 2015, 21, 243.	1.8	3
51	Protein folding with the adaptive tempering Monte Carlo method. Molecular Simulation, 2007, 33, 577-582.	2.0	2
52	Data Mining of Molecular Simulations Suggest Key Amino Acid Residues for Aggregation, Signaling and Drug Action. Biomolecules, 2021, 11, 1541.	4.0	2
53	Partitioning of AÎ² Peptide Fragments into Bloodâ€“Brain Barrier Mimetic Bilayer. Journal of Physical Chemistry B, 2021, 125, 2658-2676.	2.6	1