# 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 | 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 |
| 2 | Mechanisms of Binding of Antimicrobial Peptide PGLa to DMPC/DMPG Membrane. Journal of Chemical Information and Modeling, 2022, 62, 1525-1537. | 5.4 | 5 |
| 3 | Predicting Genetic Variation Severity Using Machine Learning to Interpret Molecular Simulations. Biophysical Journal, 2021, 120, 189-204. | 0.5 | 15 |
| 4 | Partitioning of AÎ² Peptide Fragments into Bloodâ€“Brain Barrier Mimetic Bilayer. Journal of Physical Chemistry B, 2021, 125, 2658-2676. | 2.6 | 1 |
| 5 | Met35 Oxidation Hinders AÎ²25-35 Peptide Aggregation within the Dimyristoylphosphatidylcholine Bilayer. ACS Chemical Neuroscience, 2021, 12, 3225-3236. | 3.5 | 7 |
| 6 | Data Mining of Molecular Simulations Suggest Key Amino Acid Residues for Aggregation, Signaling and Drug Action. Biomolecules, 2021, 11, 1541. | 4.0 | 2 |
| 7 | Phosphorylation Promotes AÎ²25â€“35 Peptide Aggregation within the DMPC Bilayer. ACS Chemical Neuroscience, 2020, 11, 3430-3441. | 3.5 | 8 |
| 8 | 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 |
| 9 | Three Popular Force Fields Predict Consensus Mechanism of Amyloid Î² Peptide Binding to the Dimyristoylglycerophosphocholine Bilayer. Journal of Chemical Information and Modeling, 2020, 60, 2282-2293. | 5.4 | 11 |
| 10 | De novo aggregation of Alzheimerâ€™s AÎ²25-35 peptides in a lipid bilayer. Scientific Reports, 2019, 9, 7161. | 3.3 | 21 |
| 11 | Methionine Oxidation Changes the Mechanism of AÎ² Peptide Binding to the DMPC Bilayer. Scientific Reports, 2019, 9, 5947. | 3.3 | 13 |
| 12 | Do Cholesterol and Sphingomyelin Change the Mechanism of AÎ²<sub>25â€“35</sub> Peptide Binding to Zwitterionic Bilayer?. Journal of Chemical Information and Modeling, 2019, 59, 5207-5217. | 5.4 | 7 |
| 13 | 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 |
| 14 | Binding of Cytotoxic AÎ²25â€“35 Peptide to the Dimyristoylphosphatidylcholine Lipid Bilayer. Journal of Chemical Information and Modeling, 2018, 58, 1053-1065. | 5.4 | 28 |
| 15 | Inclusion of lipopeptides into the DMPC lipid bilayers prevents AÎ² peptide insertion. Physical Chemistry Chemical Physics, 2017, 19, 10087-10098. | 2.8 | 6 |
| 16 | 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 |
| 17 | Is the Conformational Ensemble of Alzheimerâ€™s AÎ²10-40 Peptide Force Field Dependent?. PLoS Computational Biology, 2017, 13, e1005314. | 3.2 | 22 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | Molecular Mechanisms of Alzheimerâ€™s Biomarker FDDNP Binding to AÎ² Amyloid Fibril. Journal of Physical Chemistry B, 2015, 119, 11568-11580. | 2.6 | 14 |
| 21 | Calcium Enhances Binding of A Î² Monomer to DMPC Lipid Bilayer. Biophysical Journal, 2015, 108, 1807-1818. | 0.5 | 16 |
| 22 | Greedy replica exchange algorithm for heterogeneous computing grids. Journal of Molecular Modeling, 2015, 21, 243. | 1.8 | 3 |
| 23 | 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 |
| 24 | Binding of AÎ² peptide creates lipid density depression in DMPC bilayer. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2678-2688. | 2.6 | 22 |
| 25 | Revealing Hidden Helix Propensity in AÎ² Peptides by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 12030-12038. | 2.6 | 7 |
| 26 | Binding to the lipid monolayer induces conformational transition in AÎ² monomer. Journal of Molecular Modeling, 2013, 19, 737-750. | 1.8 | 9 |
| 27 | Explicit Solvent Molecular Dynamics Simulations of AÎ² Peptide Interacting with Ibuprofen Ligands. Journal of Physical Chemistry B, 2012, 116, 12922-12932. | 2.6 | 33 |
| 28 | Molecular Interactions of Alzheimer's Biomarker FDDNP with AÎ² Peptide. Biophysical Journal, 2012, 103, 2341-2351. | 0.5 | 15 |
| 29 | Naproxen Interferes with the Assembly of AÎ² Oligomers Implicated in Alzheimer's Disease. Biophysical Journal, 2011, 100, 2024-2032. | 0.5 | 23 |
| 30 | Does amino acid sequence determine the properties of AÎ² dimer?. Journal of Chemical Physics, 2011, 135, 035103. | 3.0 | 3 |
| 31 | Binding of nonsteroidal antiâ€inflammatory drugs to AÎ² fibril. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2849-2860. | 2.6 | 30 |
| 32 | Globular state in the oligomers formed by AÎ² peptides. Journal of Chemical Physics, 2010, 132, 225101. | 3.0 | 7 |
| 33 | Molecular Dynamics Simulations of Anti-Aggregation Effect of Ibuprofen. Biophysical Journal, 2010, 98, 2662-2670. | 0.5 | 26 |
| 34 | Mapping Conformational Ensembles of AÎ² Oligomers in Molecular Dynamics Simulations. Biophysical Journal, 2010, 99, 1949-1958. | 0.5 | 41 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Interpeptide interactions induce helix to strand structural transition in AÎ² peptides. Proteins: Structure, Function and Bioinformatics, 2009, 77, 1-13. | 2.6 | 141 |
| 38 | 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 |
| 39 | Replica Exchange Simulations of the Thermodynamics of AÎ² Fibril Growth. Biophysical Journal, 2009, 96, 442-452. | 0.5 | 95 |
| 40 | Probing Energetics of AÎ² Fibril Elongation by Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 4428-4437. | 0.5 | 49 |
| 41 | Molecular Dynamics Simulations of Ibuprofen Binding to AÎ² Peptides. Biophysical Journal, 2009, 97, 2070-2079. | 0.5 | 53 |
| 42 | Probing the Effect of Amino-Terminal Truncation for AÎ²1â˜'40 Peptides. Journal of Physical Chemistry B, 2009, 113, 6692-6702. | 2.6 | 40 |
| 43 | Lattice simulations of cotranslational folding of single domain proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 925-937. | 2.6 | 18 |
| 44 | Temperature-Induced Dissociation of AÎ² Monomers from Amyloid Fibril. Biophysical Journal, 2008, 95, 1758-1772. | 0.5 | 21 |
| 45 | Dissociation of AÎ²16â€“22 Amyloid Fibrils Probed by Molecular Dynamics. Journal of Molecular Biology, 2007, 368, 1202-1213. | 4.2 | 28 |
| 46 | Mechanical Unbinding of AÎ² Peptides from Amyloid Fibrils. Journal of Molecular Biology, 2007, 373, 785-800. | 4.2 | 15 |
| 47 | Protein folding with the adaptive tempering Monte Carlo method. Molecular Simulation, 2007, 33, 577-582. | 2.0 | 2 |
| 48 | Folding of tandem-linked domains. Proteins: Structure, Function and Bioinformatics, 2007, 67, 795-810. | 2.6 | 8 |
| 49 | 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 |
| 50 | Symmetric Connectivity of Secondary Structure Elements Enhances the Diversity of Folding Pathways. Journal of Molecular Biology, 2005, 353, 1171-1186. | 4.2 | 50 |
| 51 | 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 |
| 52 | Dissecting the Assembly of AÎ²16â€“22 Amyloid Peptides into Antiparallel Î² Sheets. Structure, 2003, 11, 295-307. | 3.3 | 360 |
| 53 | Protein folding kinetics: timescales, pathways and energy landscapes in terms of sequence-dependent properties. Folding & Design, 1997, 2, 1-22. | 4.5 | 390 |