# Man Hoang Viet

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6657899/publications.pdf

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|---|---|---|---|
| 58 papers | 1,715 citations | 304368 22 h-index | 301761 39 g-index |
| 62 all docs | 62 docs citations | 62 times ranked | 1816 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Recent progress in general force fields of small molecules. Current Opinion in Structural Biology, 2022, 72, 187-193. | 2.6 | 15 |
| 2 | A multiple-step in silico screening protocol to identify allosteric inhibitors of Spikeâ€“hACE2 binding. Physical Chemistry Chemical Physics, 2022, 24, 4305-4316. | 1.3 | 6 |
| 3 | Elastic moduli of normal and cancer cell membranes revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 6225-6237. | 1.3 | 10 |
| 4 | Joint Computational/Cell-Based Approach for Screening Inhibitors of Tau Oligomerization: A Proof-of-Concept Study. Journal of Alzheimer's Disease, 2022, 89, 107-119. | 1.2 | 2 |
| 5 | Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. Journal of Chemical Theory and Computation, 2021, 17, 1086-1097. | 2.3 | 16 |
| 6 | Nonequilibrium molecular dynamics simulations of infrared laser-induced dissociation of a tetrameric AÎ²42 Î²-barrel in a neuronal membrane model. Chemistry and Physics of Lipids, 2021, 234, 105030. | 1.5 | 2 |
| 7 | Molecular conformations and dynamics of nucleotide repeats associated with neurodegenerative diseases: double helices and CAG hairpin loops. Computational and Structural Biotechnology Journal, 2021, 19, 2819-2832. | 1.9 | 11 |
| 8 | Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. Journal of Cheminformatics, 2021, 13, 11. | 2.8 | 1 |
| 9 | Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. Briefings in Bioinformatics, 2021, 22, . | 3.2 | 17 |
| 10 | In silico binding profile characterization of SARS-CoV-2 spike protein and its mutants bound to human ACE2 receptor. Briefings in Bioinformatics, 2021, 22, . | 3.2 | 22 |
| 11 | Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. Langmuir, 2021, 37, 7945-7954. | 1.6 | 5 |
| 12 | Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of PHF6 Peptide of Tau Protein. Journal of Chemical Theory and Computation, 2021, 17, 6458-6471. | 2.3 | 23 |
| 13 | Molecular mechanism of ultrasound interaction with a blood brain barrier model. Journal of Chemical Physics, 2020, 153, 045104. | 1.2 | 15 |
| 14 | A fast and high-quality charge model for the next generation general AMBER force field. Journal of Chemical Physics, 2020, 153, 114502. | 1.2 | 195 |
| 15 | Infrared Laser-Induced Amyloid Fibril Dissociation: A Joint Experimental/Theoretical Study on the GNNQQNY Peptide. Journal of Physical Chemistry B, 2020, 124, 6266-6277. | 1.2 | 16 |
| 16 | Prediction of the Binding Affinities and Selectivity for CB1 and CB2 Ligands Using Homology Modeling, Molecular Docking, Molecular Dynamics Simulations, and MM-PBSA Binding Free Energy Calculations. ACS Chemical Neuroscience, 2020, 11, 1139-1158. | 1.7 | 38 |
| 17 | Tau R3â€“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. | 1.2 | 30 |
| 18 | Fast, Accurate, and Reliable Protocols for Routine Calculations of Proteinâ€“Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619. | 1.6 | 74 |

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|---|---|---|---|
| 19 | Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of AÎ² Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935. | 2.3 | 7 |
| 20 | Nonequilibrium atomistic molecular dynamics simulation of tubular nanomotor propelled by bubble propulsion. Journal of Chemical Physics, 2019, 151, 024103. | 1.2 | 4 |
| 21 | Molecular Mechanism and Kinetics of Amyloid-Î²<sub>42</sub> Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658. | 1.7 | 13 |
| 22 | Prediction of Drugâ€“Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. Drugs in R and D, 2019, 19, 297-305. | 1.1 | 17 |
| 23 | Interaction mechanism between the focused ultrasound and lipid membrane at the molecular level. Journal of Chemical Physics, 2019, 150, 215101. | 1.2 | 11 |
| 24 | New application of in silico methods in identifying mechanisms of action and key components of anti-cancer herbal formulation YIV-906 (PHY906). Physical Chemistry Chemical Physics, 2019, 21, 23501-23513. | 1.3 | 9 |
| 25 | Calculate proteinâ€“ligand binding affinities with the extended linear interaction energy method: application on the Cathepsin S set in the D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 105-117. | 1.3 | 27 |
| 26 | Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of AÎ²<sub>16â€“22</sub> Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452. | 2.3 | 102 |
| 27 | Molecular Mechanism of the Cell Membrane Pore Formation Induced by Bubble Stable Cavitation. Journal of Physical Chemistry B, 2019, 123, 71-78. | 1.2 | 25 |
| 28 | Structure and Dynamics of DNA and RNA Double Helices Obtained from the CCG and GGC Trinucleotide Repeats. Journal of Physical Chemistry B, 2018, 122, 4491-4512. | 1.2 | 16 |
| 29 | E-motif formed by extrahelical cytosine bases in DNA homoduplexes of trinucleotide and hexanucleotide repeats. Nucleic Acids Research, 2018, 46, 942-955. | 6.5 | 19 |
| 30 | Rayleigh-Plesset equation of the bubble stable cavitation in water: A nonequilibrium all-atom molecular dynamics simulation study. Journal of Chemical Physics, 2018, 148, . | 1.2 | 22 |
| 31 | Breaking down cellulose fibrils with a mid-infrared laser. Cellulose, 2018, 25, 5553-5568. | 2.4 | 8 |
| 32 | Conformational Ensembles of the Wild-Type and S8C AÎ²1â€“42 Dimers. Journal of Physical Chemistry B, 2017, 121, 2434-2442. | 1.2 | 31 |
| 33 | High-Resolution Structures of the Amyloid-Î² 1â€“42 Dimers from the Comparison of Four Atomistic Force Fields. Journal of Physical Chemistry B, 2017, 121, 5977-5987. | 1.2 | 120 |
| 34 | Structure and Dynamics of DNA and RNA Double Helices of CAG and GAC Trinucleotide Repeats. Biophysical Journal, 2017, 113, 19-36. | 0.2 | 19 |
| 35 | AÎ²41 Aggregates More Like AÎ²40 than Like AÎ²42: In Silico and in Vitro Study. Journal of Physical Chemistry B, 2016, 120, 7371-7379. | 1.2 | 13 |
| 36 | Comparative melting and healing of B-DNA and Z-DNA by an infrared laser pulse. Journal of Chemical Physics, 2016, 144, 145101. | 1.2 | 6 |

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|---|---|---|---|
| 37 | Nonequilibrium all-atom molecular dynamics simulation of the bubble cavitation and application to dissociate amyloid fibrils. Journal of Chemical Physics, 2016, 145, 174113. | 1.2 | 30 |
| 38 | Contrasting Roles of Asparagine and Glutamine in the Aggregation of Prion-Like Proteins. Biophysical Journal, 2016, 110, 214a-215a. | 0.2 | 0 |
| 39 | Stability and Ion Distributions Around Left- and Right-Handed DNA and RNA Duplexes: A Comparative Study. Biophysical Journal, 2016, 110, 407a. | 0.2 | 1 |
| 40 | Structural Determinants of Polyqlutamine Protofibrils and Crystallites. Biophysical Journal, 2016, 110, 215a. | 0.2 | 0 |
| 41 | Picosecond infrared laser-induced all-atom nonequilibrium molecular dynamics simulation of dissociation of viruses. Physical Chemistry Chemical Physics, 2016, 18, 11951-11958. | 1.3 | 9 |
| 42 | Amyloid Properties of Asparagine and Glutamine in Prion-like Proteins. ACS Chemical Neuroscience, 2016, 7, 576-587. | 1.7 | 30 |
| 43 | Picosecond dissociation of amyloid fibrils with infrared laser: A nonequilibrium simulation study. Journal of Chemical Physics, 2015, 143, 155101. | 1.2 | 41 |
| 44 | Structural Determinants of Polyglutamine Protofibrils and Crystallites. ACS Chemical Neuroscience, 2015, 6, 632-645. | 1.7 | 12 |
| 45 | High performance p-type segmented leg of misfit-layered cobaltite and half-Heusler alloy. Energy Conversion and Management, 2015, 99, 20-27. | 4.4 | 23 |
| 46 | In Silico and in Vitro Study of Binding Affinity of Tripeptides to Amyloid Î² Fibrils: Implications for Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2015, 119, 5145-5155. | 1.2 | 30 |
| 47 | Picosecond melting of peptide nanotubes using an infrared laser: a nonequilibrium simulation study. Physical Chemistry Chemical Physics, 2015, 17, 27275-27280. | 1.3 | 14 |
| 48 | Communication: Multiple atomistic force fields in a single enhanced sampling simulation. Journal of Chemical Physics, 2015, 143, 021101. | 1.2 | 9 |
| 49 | Effects of Water Models on Binding Affinity: Evidence from All-Atom Simulation of Binding of Tamiflu to A/H5N1 Neuraminidase. Scientific World Journal, The, 2014, 2014, 1-14. | 0.8 | 42 |
| 50 | Tripeptides Screening Report: Proline is Important for AÎ² Fibrils Depolymerization. Biophysical Journal, 2014, 106, 55a-56a. | 0.2 | 0 |
| 51 | Effect of Taiwan Mutation (D7H) on Structures of Amyloid-Î² Peptides: Replica Exchange Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 8972-8981. | 1.2 | 36 |
| 52 | Effect of the English Familial Disease Mutation (H6R) on the Monomers and Dimers of AÎ²40 and AÎ²42. ACS Chemical Neuroscience, 2014, 5, 646-657. | 1.7 | 49 |
| 53 | Effect of the Tottori Familial Disease Mutation (D7N) on the Monomers and Dimers of AÎ²<sub>40</sub> and AÎ²<sub>42</sub>. ACS Chemical Neuroscience, 2013, 4, 1446-1457. | 1.7 | 83 |
| 54 | Discovery of Dihydrochalcone as Potential Lead for Alzheimerâ€™s Disease: In Silico and In Vitro Study. PLoS ONE, 2013, 8, e79151. | 1.1 | 33 |

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|---|---|---|---|
| 55 | Amyloid peptide AÎ²40 inhibits aggregation of AÎ²42: Evidence from molecular dynamics simulations. Journal of Chemical Physics, 2012, 136, 245105. | 1.2 | 38 |
| 56 | Inhibition of Aggregation of Amyloid Peptides by Beta-Sheet Breaker Peptides and Their Binding Affinity. Journal of Physical Chemistry B, 2011, 115, 7433-7446. | 1.2 | 173 |
| 57 | Top Leads for Swine Influenza A/H1N1 Virus Revealed by Steered Molecular Dynamics Approach. Journal of Chemical Information and Modeling, 2010, 50, 2236-2247. | 2.5 | 84 |
| 58 | Studying submicrosecond protein folding kinetics using a photolabile caging strategy and timeâ€resolved photoacoustic calorimetry. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2973-2983. | 1.5 | 8 |