Novelty Assessment Report

Paper: Unified Biomolecular Trajectory Generation via Pretrained Variational Bridge
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Abstract

Molecular Dynamics (MD) simulations provide a fundamental tool for characterizing molecular behavior at full atomic resolution, but their applicability is severely constrained by the computational cost. To address this, a surge of deep generative models has recently emerged to learn dynamics at coarsened timesteps for efficient trajectory generation, yet they either generalize poorly across systems or, due to limited molecular diversity of trajectory data, fail to fully exploit structural information to improve generative fidelity. Here, we present the Pretrained Variational Bridge (PVB) in an encoder-decoder fashion, which maps the initial structure into a noised latent space and transports it toward stage-specific targets through augmented bridge matching. This unifies training on both single-structure and paired trajectory data, enabling consistent use of cross-domain structural knowledge across training stages. Moreover, for protein-ligand complexes, we further introduce a reinforcement learning-based optimization via adjoint matching that speeds progression toward the holo state, which supports efficient post-optimization of docking poses. Experiments on proteins and protein-ligand complexes demonstrate that PVB faithfully reproduces thermodynamic and kinetic observables from MD while delivering stable and efficient generative dynamics.

Core Task Landscape

This paper addresses: **Accelerating Molecular Dynamics Simulations through Deep Generative Modeling**

A total of **50 papers** were analyzed and organized into a taxonomy with **20 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Deep Generative Models for Conformational Sampling and Trajectory Generation**
- **Enhanced Sampling and Free Energy Calculation with Deep Learning**
- **Machine Learning Force Fields and Accelerated Simulation Engines**
- **Deep Learning for Molecular Property Prediction and Analysis**
- **Deep Generative Models for Drug Discovery and Molecular Design**
- **Reviews, Perspectives, and Methodological Frameworks**

Complete Taxonomy Tree

- Accelerating Molecular Dynamics Simulations through Deep Generative Modeling Survey Taxonomy
- Deep Generative Models for Conformational Sampling and Trajectory Generation
  - Diffusion-Based Generative Models for Biomolecular Dynamics ★ (5 papers)
  - [0] Unified Biomolecular Trajectory Generation via Pretrained Variational Bridge (Anon et al., 2026) View paper
  - [1] DynamicBind: predicting ligand-specific protein-ligand complex structure with a deep equivariant generative model (Wei, 2024) View paper
  - [11] How good is generative diffusion model for enhanced sampling of protein conformations across scales and in all-atom resolution? (Palash, 2025) View paper
  - [26] â¦ Intelligence in Predicting Membrane Partitioning of Drugs: Combining Denoising Diffusion Probabilistic Models and MD Simulations Reduces the Computational Cost â¦ (P Obi, 2024) View paper
  - [37] Dynamicsdiffusion: Generating and rare event sampling of molecular dynamic trajectories using diffusion models (M Petersen, 2023) View paper
  - Autoencoder and Latent Space Models for Conformational Ensembles (4 papers)
  - [9] Sampling conformational ensembles of highly dynamic proteins via generative deep learning (T Ruzmetov, 2025) View paper
  - [14] Deep generative modeling of temperature-dependent structural ensembles of proteins (Giacomo Janson, 2025) View paper
  - [28] Reinforced molecular dynamics: Physics-infused generative machine learning model explores CRBN activation process (IstvÃ¡n KolossvÃ¡ry, 2025) View paper
  - [31] Phanto-IDP: compact model for precise intrinsically disordered protein backbone generation and enhanced sampling (Junjie Zhu, 2023) View paper
  - Generative Markov State Models and Trajectory Synthesis (4 papers)
  - [30] Simple synthetic molecular dynamics for efficient trajectory generation (Russo, 2022) View paper
  - [40] Generative modeling of molecular dynamics trajectories (Bonnie Berger, 2024) View paper
  - [41] Deep generative markov state models (Hao Wu, 2018) View paper
  - [50] Learning molecular dynamics: predicting the dynamics of glasses by a machine learning simulator (Han Liu, 2023) View paper
  - Comparative Studies and Benchmarking of Generative Frameworks (1 papers)
  - [35] A comparison of probabilistic generative frameworks for molecular simulations. (Richard John, 2025) View paper
- Enhanced Sampling and Free Energy Calculation with Deep Learning
  - Gaussian-Accelerated Molecular Dynamics with Deep Learning (7 papers)

- [16] GLOW: A Workflow Integrating Gaussian-Accelerated Molecular Dynamics and Deep Learning for Free Energy Profiling. (H. Do, 2022) View paper
- [17] â¦ Interaction Mechanisms of Peptide and Non-Peptide Inhibitors with MDM2 Using Gaussian-Accelerated Molecular Dynamics Simulations and Deep Learning (W Yang, 2024) View paper
- [23] Insights into the Interaction Mechanisms of Peptide and Non-Peptide Inhibitors with MDM2 Using Gaussian-Accelerated Molecular Dynamics Simulations and Deep Learning (Wanchun Yang, 2024) View paper
- [32] Molecular mechanism underlying effect of D93 and D289 protonation states on inhibitor-BACE1 binding: exploration from multiple independent Gaussian accelerated molecular dynamics and deep learning (Du J, 2024) View paper
- [33] â¦ of D93 and D289 protonation states on inhibitor-BACE1 binding: exploration from multiple independent Gaussian accelerated molecular dynamics and deep learning (J Du, 2024) View paper
- [42] Unveiling Conformational States of CDK6 Caused by Binding of Vcyclin Protein and Inhibitor by Combining Gaussian Accelerated Molecular Dynamics and Deep Learning (Lu Zhao, 2024) View paper
- [43] â¦ States of CDK6 Caused by Binding of Vcyclin Protein and Inhibitor by Combining Gaussian Accelerated Molecular Dynamics and Deep Learning (L Zhao, 2024) View paper
- Deep Generative Models for Unbiasing and Reweighting Enhanced Sampling (3 papers)
- [10] Unbiasing Enhanced Sampling on a High-Dimensional Free Energy Surface with a Deep Generative Model (Yikai Liu, 2024) View paper
- [19] Unbiasing Enhanced Sampling on a High-dimensional Free Energy Surface with Deep Generative Model (Liu Yikai, 2023) View paper
- [29] â¦ Molecular Unnormalized Distributions With Deep Generative Models Toward the Acceleration of Molecular Design and Conformational Sampling With Deep â¦ (Diez, 2024) View paper
- Deep Boosted Molecular Dynamics and Gaussian Boost Potentials (2 papers)
- [15] Deep Boosted Molecular Dynamics (DBMD): Accelerating molecular simulations with Gaussian boost potentials generated using probabilistic Bayesian deep neural network (N. Hung, 2023) View paper
- [21] Deep Boosted Molecular Dynamics: Accelerating Molecular Simulations with Gaussian Boost Potentials Generated Using Probabilistic Bayesian Deep Neural Network. (H. Do, 2023) View paper
- Deep Learning Collective Variables for Enhanced Sampling (1 papers)
- [46] Deep learning path-like collective variable for enhanced sampling molecular dynamics. (FrÃ¶hlking, 2024) View paper

- Machine Learning Force Fields and Accelerated Simulation Engines
  - Deep Neural Network Potentials for Molecular Dynamics (2 papers)
  - [20] Accurate and efficient molecular dynamics based on machine learning and non von Neumann architecture (Pinghui Mo, 2022) View paper
  - [45] Transition State Searching Accelerated by Deep Learning Potential (Bowen Li, 2024) View paper
  - Learning Effective Coarse-Grained Dynamics (2 papers)
  - [13] Accelerated simulations of molecular systems through learning of effective dynamics (Pantelis R. Vlachas, 2021) View paper
  - [25] Accelerated Simulations of Molecular Systems through Learning of their Effective Dynamics (Vlachas, 2022) View paper
  - Transferable Generative Models for Multi-Timescale Dynamics (1 papers)
  - [27] Transferable Generative Models Bridge Femtosecond to Nanosecond Time-Step Molecular Dynamics (Schreiner, 2025) View paper
- Deep Learning for Molecular Property Prediction and Analysis
  - Unsupervised Deep Learning for MD Trajectory Analysis (1 papers)
  - [8] Unsupervised deep learning for molecular dynamics simulations: a novel analysis of proteinâ□ligand interactions in SARS-CoV-2 Mpro (Jessica Mustali, 2023) View paper
  - Deep Learning for Molecular Property and Spectra Prediction (2 papers)
  - [2] Accelerating Molecular Vibrational Spectra Simulations with a Physically Informed Deep Learning Model. (Yuzhuo Chen, 2024) View paper
  - [12] Prediction of Water Diffusion in Wide Varieties of Polymers with All-Atom Molecular Dynamics Simulations and Deep Generative Models (Ryo Kawada, 2022) View paper
  - Deep Learning for Solvation and Membrane Partitioning (2 papers)
  - [6] Calculation of solvation force in molecular dynamics simulation by deep-learning method (Jun Liao, 2024) View paper
  - [34] Application of Generative Artificial Intelligence in Predicting Membrane Partitioning of Drugs: Combining Denoising Diffusion Probabilistic Models and MD Simulations Reduces the Computational Cost to One-Third. (P. Obi, 2024) View paper
  - Deep Learning for Microstructure Evolution Prediction (1 papers)
  - [18] Prediction of microstructure evolution at the atomic scale by deep generative model in combination with recurrent neural networks (Kohei Sase, 2023) View paper
- Deep Generative Models for Drug Discovery and Molecular Design
  - Generative Models for De Novo Molecular Design (2 papers)
  - [3] Deep generative molecular design reshapes drug discovery (Xiangxiang Zeng, 2022) View paper
  - [38] Improving drug discovery with a hybrid deep generative model using reinforcement learning trained on a Bayesian docking approximation (Youjin Xiong, 2023) View paper
  - Generative Models for Peptide and Protein Design (2 papers)
  - [5] De novo carbon monoxide dehydrogenase and carbonic anhydrase using molecular dynamics and deep generative model (Ruei-En Hu, 2025) View paper
  - [36] Accelerated NLRP3 inflammasome-inhibitory peptide design using a recurrent neural network model and molecular dynamics simulations (Bilal Ahmad, 2023) View paper
  - Generative Models for Virtual Screening and Inhibitor Identification (2 papers)
  - [7] Identification of STAT3 phosphorylation inhibitors using generative deep learning, virtual screening, molecular dynamics simulations, and biological evaluation for non â¦ (W Cai, 2025) View paper
  - [22] Identification of potential PIM-2 inhibitors via ligand-based generative models, molecular docking and molecular dynamics simulations (Tianli Qin, 2024) View paper
  - Generative AI for Architected Material Design (1 papers)
  - [44] Generative AI model trained by molecular dynamics for rapid mechanical design of architected graphene (Milad Masrouri, 2024) View paper
- Reviews, Perspectives, and Methodological Frameworks (6 papers)
  - [4] Generation of protein dynamics by machine learning (Giacomo Janson, 2025) View paper

- [24] Generative AI for computational chemistry: A roadmap to predicting emergent phenomena (P. Tiwary, 2025) View paper
- [39] Generative artificial intelligence for computational chemistry: a roadmap to predicting emergent phenomena (Tiwary, 2024) View paper
- [47] Author Correction: Accelerated antimicrobial discovery via deep generative models and molecular dynamics simulations (Payel Das, 2021) View paper
- [48] Deep learning tools to accelerate antibiotic discovery (Angela Cesaro, 2023) View paper
- [49] Machine Learning Driven Drug Discovery: Accelerating the Identification of Novel Therapeutics through Deep Generative Models and Molecular Simulation (Hanafi Musa Olayinka, 2025) View paper

Narrative

Core task: accelerating molecular dynamics simulations through deep generative modeling. The field has organized itself into several major branches that reflect different strategies for leveraging deep learning to overcome the timescale limitations of traditional MD. One branch focuses on conformational sampling and trajectory generation, where models learn to produce realistic molecular configurations or entire dynamical pathways without exhaustive simulation. Another branch emphasizes enhanced sampling and free energy calculation, using neural networks to identify collective variables or reweight biased simulations. A third branch develops machine learning force fields that replace expensive quantum calculations with fast learned potentials, while additional branches address property prediction, drug discovery applications, and methodological reviews. Representative works such as Diffusion Protein Conformations[11] and Dynamics Diffusion[37] illustrate how diffusion-based architectures have become prominent tools for generating biomolecular ensembles, whereas efforts like Deep Boosted MD[15] and Unbiasing Enhanced Sampling[10] show how learning can guide or correct biased sampling schemes.

Within the conformational sampling branch, diffusion-based generative models have emerged as a particularly active line of work, balancing the need for physical realism with computational efficiency. These methods must navigate trade-offs between sampling speed, conformational diversity, and adherence to underlying energy landscapes. Biomolecular Variational Bridge[0] sits squarely in this diffusion-focused cluster, sharing methodological DNA with Diffusion Protein Conformations[11] and Dynamics Diffusion[37], which similarly apply diffusion frameworks to generate protein or molecular trajectories. Compared to DynamicBind[1], which targets dynamic protein-ligand binding, Biomolecular Variational Bridge[0] appears to emphasize broader conformational exploration rather than binding-specific dynamics. Meanwhile, Membrane Partitioning Diffusion[26] applies diffusion models to membrane systems, highlighting how these generative techniques are being adapted across diverse biomolecular contexts. The central challenge remains ensuring that generated samples faithfully represent thermodynamic ensembles while achieving meaningful speedups over conventional simulation.

Related Works in Same Category

The following **4 sibling papers** share the same taxonomy leaf node with the original paper:

1. DynamicBind: predicting ligand-specific protein-ligand complex structure with a deep equivariant generative model

Authors: Lu Wei | **Year/Venue**: 2024 | **URL**: View paper

Abstract

Proteins often function by changing conformations upon ligand binding. Efficient structural modelling of these interactions, crucial for drug discovery, is limited: here the authors address this with DynamicBind, a diffusion-based deep generative model. While significant advances have been made in predicting static protein structures, the inherent dynamics of proteins, modulated by ligands, are crucial for understanding protein function and facilitating drug discovery. Traditional docking method...

Relationship Analysis

Both papers belong to the category of diffusion-based generative models for biomolecular dynamics, employing denoising diffusion or flow matching techniques to generate conformational ensembles. They overlap in addressing protein-ligand complex dynamics and accelerating conformational sampling beyond traditional MD simulations. However, the original paper (PVB) focuses on unified trajectory generation across training stages using augmented bridge matching with encoder-decoder architecture and RL-based optimization for temporal evolution, while the candidate paper (DynamicBind) specifically targets ligand-specific protein conformational changes for docking applications using equivariant geometric diffusion networks without explicit trajectory generation or temporal dynamics modeling.

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2. How good is generative diffusion model for enhanced sampling of protein conformations across scales and in all-atom resolution?

Authors: Bera Palash | **Year/Venue**: 2025 | **URL**: View paper

Abstract

Molecular dynamics (MD) simulations are fundamental for probing the structural dynamics of biomolecules, yet their efficiency is limited by the high computational cost of exploring long-timescale events. Generative machine learning (ML) models, particularly the Denoising Diffusion Probabilistic Model (DDPM), offer an emerging strategy to enhance conformational sampling. In this study, we evaluate the capabilities and limitations of DDPM in generating atomistically accurate conformational ensembl...

Relationship Analysis

Both papers belong to the diffusion-based generative models category for biomolecular dynamics, employing denoising diffusion probabilistic models to generate conformational ensembles. While the original paper (PVB) focuses on unified trajectory generation across molecular domains using an encoder-decoder architecture with bridge matching and RL-based optimization for protein-ligand complexes, the candidate paper evaluates standard DDPM capabilities and limitations for enhanced sampling across proteins of varying sizes and disorder levels (from folded proteins to IDPs), without the unified cross-domain framework or RL components. The key distinction is that PVB proposes a novel pretrained variational bridge method with trajectory generation capabilities, whereas the candidate paper benchmarks existing DDPM approaches for conformational ensemble generation.

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3. â¦ Intelligence in Predicting Membrane Partitioning of Drugs: Combining Denoising Diffusion Probabilistic Models and MD Simulations Reduces the Computational Cost â¦

Authors: P Obi, JB Gc, C Mariasoosai, A Diyaolu | **Year/Venue**: 2024 | **URL**: View paper

Abstract

â¦ Molecular dynamics (MD) simulations, including enhanced â¦), a generative AI method, to US simulation data reduces the â¦) data from the US simulations and reproduced the complete â¦

Relationship Analysis

Both papers belong to the diffusion-based generative models category for biomolecular dynamics, employing denoising diffusion probabilistic models to accelerate molecular simulations. The candidate paper focuses on combining diffusion models with umbrella sampling (US) simulations specifically for predicting membrane partitioning of drugs, using generative AI to reduce computational costs

of enhanced sampling methods. In contrast, the original paper (PVB) presents a unified encoder-decoder framework with augmented bridge matching for general trajectory generation across diverse biomolecular systems (proteins and protein-ligand complexes), incorporating reinforcement learning for accelerated exploration of holo states rather than focusing on membrane partitioning tasks.

4. Dynamicsdiffusion: Generating and rare event sampling of molecular dynamic trajectories using diffusion models

Authors: M Petersen, G Roig, R Covino | **Year/Venue**: 2023 | **URL**: View paper

Abstract

â¦ molecular dynamics trajectories. We hope this work will motivate a new generation of generative modeling for the study of molecular dynamics. â¦ the first deep generative model to â¦

Relationship Analysis

Both papers belong to the diffusion-based generative models category, employing denoising diffusion probabilistic models to generate biomolecular trajectories and conformational ensembles. They overlap in using diffusion models for molecular dynamics trajectory generation with coarse-grained timesteps to accelerate simulations beyond traditional MD integration. The key differences are that the original paper (PVB) introduces an encoder-decoder architecture with augmented bridge matching for unified pretraining/finetuning and RL-based optimization for protein-ligand complexes, while the candidate paper (DynamicsDiffusion) focuses on standard DDPM with inpainting techniques for rare event sampling and does not incorporate pretraining or RL components.

Contributions Analysis

Overall novelty summary. The paper introduces a Pretrained Variational Bridge (PVB) framework that unifies training on single-structure and paired trajectory data through augmented bridge matching, with reinforcement learning-based optimization for protein-ligand complexes. It resides in the 'Diffusion-Based Generative Models for Biomolecular Dynamics' leaf, which contains five papers including the original work. This represents a moderately populated research direction within the broader conformational sampling branch, suggesting active but not overcrowded exploration of diffusion-based approaches for molecular trajectory generation.

The taxonomy reveals neighboring leaves focused on autoencoder-based conformational ensembles, generative Markov state models, and comparative benchmarking studies. The paper's bridge matching approach connects to the diffusion paradigm shared by sibling works like Diffusion Protein Conformations and Dynamics Diffusion, yet diverges by explicitly unifying cross-domain structural knowledge across training stages. The scope note clarifies this leaf excludes VAE-based or GAN-based methods, positioning the work firmly within the diffusion modeling tradition while the reinforcement learning component introduces elements typically associated with optimization-focused branches.

Among twelve candidates examined across three contributions, no clearly refutable prior work was identified. The unified training framework examined one candidate with no refutations, the RL-based adjoint matching examined one candidate with no refutations, and the cross-domain trajectory generation demonstration examined ten candidates with no refutations. This limited search scope—twelve papers from semantic retrieval—suggests the specific combination of pretrained variational bridges with adjoint matching for protein-ligand systems may occupy a relatively unexplored niche, though the absence of refutations does not confirm comprehensive novelty given the constrained candidate pool.

Based on top-twelve semantic matches, the work appears to introduce distinctive methodological elements within an active research area. The analysis covers diffusion-based trajectory generation but does not exhaustively survey all enhanced sampling or force field approaches that might address similar acceleration goals through different paradigms. The taxonomy structure indicates this sits at the intersection of generative modeling and molecular dynamics, where rapid methodological evolution makes definitive novelty assessments challenging without broader literature coverage.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: Pretrained Variational Bridge (PVB) with unified training framework

Description: The authors introduce PVB, which uses an encoder-decoder architecture combined with augmented bridge matching to create a unified objective for pretraining on single-structure data and finetuning on MD trajectory pairs. This design enables consistent exploitation of cross-domain structural knowledge across training stages.

This contribution was assessed against **1 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Multimodal Pre-training Models of Molecular Representation for Drug Discovery

URL: View paper

Brief Assessment

Multimodal Molecular Representation[51] focuses on multimodal pre-training for drug discovery using transformers and graph neural networks for molecular representation learning, not encoder-decoder architectures with bridge matching for molecular dynamics trajectory generation.

Contribution 2: RL-based finetuning via adjoint matching for protein-ligand complexes

Description: The authors develop a reinforcement learning finetuning method using adjoint matching and stochastic optimal control. This approach modulates the generative distribution with explicit reward functions to accelerate progression toward protein-ligand holo states, enabling efficient post-optimization of docking poses.

This contribution was assessed against **1 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Process Optimal Planning and Product Design through Deep Reinforcement Learning

URL: View paper

Brief Assessment

Process Optimal Planning[52] focuses on energy management systems and molecular fragment synthesis for drug discovery, not protein-ligand docking optimization or trajectory generation using stochastic optimal control with adjoint matching.

Contribution 3: Demonstration of stable and efficient cross-domain trajectory generation

Description: The authors show that PVB faithfully reproduces thermodynamic and kinetic observables from molecular dynamics simulations across protein monomers and protein-ligand complexes, while providing more stable trajectory generation compared to baseline methods.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Enhanced Sampling, Public Dataset and Generative Model for Drug-Protein Dissociation Dynamics

URL: View paper

Brief Assessment

Drug Protein Dissociation[59] focuses on drug-protein dissociation dynamics using enhanced sampling (metadynamics) and generates trajectories for specific dissociation processes. The original paper addresses general biomolecular trajectory generation across protein monomers and protein-ligand complexes with coarse-grained timesteps, emphasizing thermodynamic/kinetic fidelity and stability. These are distinct technical approaches and application domains.

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2. Accurate prediction of the kinetic sequence of physicochemical states using generative artificial intelligence

URL: View paper

Brief Assessment

Kinetic Sequence Prediction[60] focuses on predicting discrete state sequences from MD trajectories using GPT-based models, not on generating continuous molecular trajectories across protein domains. The candidate does not address cross-domain trajectory generation or compare stability metrics.

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3. Scalable emulation of protein equilibrium ensembles with generative deep learning

URL: View paper

Brief Assessment

Protein Ensemble Emulation[53] focuses on generating independent protein structures (i.i.d. samples) from equilibrium ensembles rather than sequential trajectory generation with temporal correlations. The candidate does not address cross-domain systems or trajectory stability metrics.

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4. Deep Generative Models for Analysis and Engineering of Functional Proteins

URL: View paper

Brief Assessment

Functional Protein Engineering[54] focuses on deep generative models for protein engineering and design, not on trajectory generation methods that reproduce thermodynamic and kinetic observables from molecular dynamics simulations. The candidate addresses protein function optimization rather than dynamics simulation fidelity.

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5. Latent thermodynamic flows: unified representation learning and generative modeling of temperature-dependent behaviors from limited data

URL: View paper

Brief Assessment

Latent Thermodynamic Flows[58] focuses on temperature-dependent equilibrium distribution modeling and representation learning for molecular systems, not on cross-domain trajectory generation with coarse-grained timesteps as in the original paper.

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6. Deep generative modeling of temperature-dependent structural ensembles of proteins

URL: View paper

Brief Assessment

Temperature Dependent Ensembles[14] focuses on temperature-conditioned ensemble generation for protein monomers, not cross-domain trajectory generation across proteins and protein-ligand complexes with stability comparisons to baselines.

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7. Use of AI-methods over MD simulations in the sampling of conformational ensembles in IDPs

URL: View paper

Brief Assessment

IDP Conformational Sampling[56] focuses on intrinsically disordered proteins using AI methods as alternatives to MD simulations, not on cross-domain trajectory generation frameworks that reproduce thermodynamic and kinetic observables across protein monomers and protein-ligand complexes.

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8. Can We Extract Physics-like Energies from Generative Protein Diffusion Models?

URL: View paper

Brief Assessment

Physics Energies Diffusion[57] focuses on extracting thermodynamic potentials from diffusion models and analyzing their correspondence to physics-based energies, not on trajectory generation or reproducing kinetic/thermodynamic observables from molecular dynamics simulations.

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9. Thermodynamic Interpolation: A Generative Approach to Molecular Thermodynamics and Kinetics

URL: View paper

Brief Assessment

Thermodynamic Interpolation[55] focuses on temperature-controllable equilibrium sampling from Boltzmann distributions using normalizing flows, not on cross-domain trajectory generation or stability comparisons across protein monomers and protein-ligand complexes as demonstrated by PVB.

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10. Deep generative molecular design reshapes drug discovery

URL: View paper

Brief Assessment

Generative Molecular Design[3] focuses on drug discovery applications using deep generative models but does not address trajectory generation methods, thermodynamic/kinetic observables reproduction, or stability comparisons for molecular dynamics simulations.

Appendix: Text Similarity Detection

No high-similarity text segments were detected across any compared papers.

References

- [0] Unified Biomolecular Trajectory Generation via Pretrained Variational Bridge View paper
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- [2] Accelerating Molecular Vibrational Spectra Simulations with a Physically Informed Deep Learning Model. View paper

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