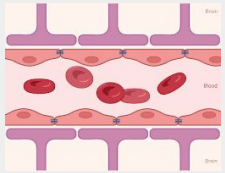
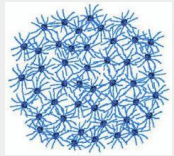
Computational Modeling of Drug Transport Across the Blood Brain Barrier

ALEX

Introduction

- The blood-brain barrier (BBB) prevents >98% of therapeutics from reaching the CNS
- Effective drug delivery to the brain is a major challenge in neuroscience and pharmacology
- Understanding transport mechanisms is key for designing therapeutics and nanoparticle carriers





Objectives

- Develop a computational framework to simulate BBB transport
- Quantify diffusion of nanoparticles and biologically derived molecules with varying size, change, and surface chemistry
- Integrate existing experimental data and stochastic modeling for predictive insights

Methods

- Computational Modeling
  - Differential equations to simulate transport kinetics
  - Stochastic diffusion models to represent molecular behavior
- Molecular Feature Analysis
  - Machine learning to identify features enhancing BBB permeability

Data
Results
Findings

Results
Conclusions

Applications

- Accelerate CNS drug development by overcoming BBB limitations
- Open-source simulation platform for research and education
- Tool in predicting targeted drug delivery, neurodegenerative disease diagnostics, and synthetic biology and biomaterials research

Citations

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