



VANDERBILT

School of Medicine Basic Sciences

Department of Pharmacology

2024 - 2025 Seminar Series

Developing a Novel In-Silico Tool for Heterochiral Macrocycle Design

Macrocycles are promising therapeutic agents, but heterochiral and non-natural building blocks complicate design. Lacking machine learning methods for heterochiral macrocycles, we developed a convolutional autoencoder to generate stable backbones. Our approach outperforms Rosetta's GenKIC. We created a custom dataset due to limited public data. The model, CyclicCAE, produces energetically stable backbones and designable structures faster than GenKIC, enabling energy minimization, MCMC-based generation of diverse structures, and inpainting with fixed anchors. This method accelerates macrocycle design, potentially expediting drug development pipelines.

May 6, 2025

4:00 PM

202 Light Hall

Host: Ben Brown



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