

Assignment#3

CH5650: Molecular Data Science and Informatic
Jan-May, 2025

Due Date: Feb 28, 2025 (Online Submission, <https://courses.iitm.ac.in/>)

1. Develop an ML model to predict the glass transition temperature of a polymer based on its monomer's chemical descriptors.
2. Develop a second ML model to predict the glass transition temperature of a polymer based on its monomer's topological descriptors.

You can use the RDKit to extract chemical and topological descriptors of a monomer. Submit your code and a PDF file with the model's description and result.