# Methodology Report

## Description of the Model

We utilized a Multi-Task Deep Neural Network (MLP) architecture implemented in PyTorch to predict all 9 ADMET properties simultaneously. The model takes 1200-dimensional molecular features (Grover Large embeddings augmented with RDKit descriptors) as input, passing them through a shared encoder block to learn generalizable representations, before branching into task-specific heads that refine predictions for each property. The network was optimized using a Weighted Masked MSE Loss function to handle missing labels and balance the learning process across diverse tasks.

## Performance comments

The model demonstrated strong generalization capabilities on the hold-out validation set, particularly excelling in ranking metrics. The high Spearman correlation scores across key tasks indicate that the multi-task approach successfully captured the relative order of molecular properties, effectively leveraging the shared representations to predict physicochemical trends even for tasks with varying data distributions.