

TABLE I
TRAINING EFFICIENCY COMPARISON ACROSS METHODOLOGIES FOR IC_{50}
DATASET

Method	Peak Memory (12.7 GB)	Training Time (s)	Storage (225.8 GB)
PGM	1.9	14	39.2
GNN	1.9	14	39.2
PGM+GNN	1.9	14	39.2
LSTM	2.0	120	39.2
chemBERT	4.3	5400	39.7

TABLE II
TRAINING EFFICIENCY COMPARISON ACROSS METHODOLOGIES FOR $\log P$
SYNTHETIC DATASET

Method	Peak Memory (12.7 GB)	Training Time (s)	Storage (225.8 GB)
PGM	1.7	55	39.2
GNN	1.7	55	39.2
PGM+GNN	1.7	55	39.2
LSTM	2.0	1920	39.2
chemBERT	7.7	18 hrs	39.7

TABLE III
TRAINING EFFICIENCY COMPARISON ACROSS METHODOLOGIES FOR $\log P$
EXP DATASET

Method	Peak Memory (12.7 GB)	Training Time (s)	Storage (225.8 GB)
PGM	1.9	11	39.2
GNN	1.9	11	39.2
PGM+GNN	1.9	11	39.2
LSTM	1.7	60	39.2
chemBERT	7.2	80	39.7

TABLE IV
TRAINING EFFICIENCY COMPARISON ACROSS METHODOLOGIES FOR FREE
ENERGY DATASET

Method	Peak Memory (12.7 GB)	Training Time (s)	Storage (225.8 GB)
PGM	2.0	23	39.2
GNN	2.0	23	39.2
PGM+GNN	2.0	23	39.2
LSTM	1.9	60	39.2
chemBERT	5.4	2820	39.7

TABLE V
TRAINING EFFICIENCY COMPARISON ACROSS METHODOLOGIES FOR
WATER SOLUBILITY DATASET

Method	Peak Memory (12.7 GB)	Training Time (s)	Storage (225.8 GB)
PGM	1.7	17	39.2
GNN	1.7	17	39.2
PGM+GNN	1.7	17	39.2
LSTM	1.9	120	39.2
chemBERT	6.0	3600	39.7