
LIST OF TABLES

3.1	The Davis (top) and KIBA (bottom) Datasets Snippet.	19
3.2	Dataset Description.	19
3.3	Molecular graph atom features.	21
3.4	Motif graph atom features.	23
3.5	Hyperparameters Configuration.	27
3.6	Parameter exploration details.	27
4.1	Parameters exploration results (Davis dataset).	30
4.2	Parameters exploration results (KIBA dataset).	31
4.3	State-of-the-art models comparison.	34
4.4	Baseline models comparison.	35
A.1	Descriptive statistics for Davis dataset	47
A.2	Descriptive statistics for KIBA dataset	48
A.3	Hyperparameters tuning results for Learning Rate (Davis dataset)	49
A.4	Hyperparameters tuning results for Batch Size (Davis dataset)	49
A.5	Hyperparameters tuning results for Learning Rate (KIBA dataset)	49
A.6	Hyperparameters tuning results for Batch Size (KIBA dataset)	49