

## Appendix

### MLPET: A Multi-Level Prompt-Enhanced Transformer for Unified Molecular

#### Property and Drug-Drug Interaction Event Prediction

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**TABLE I.** SUMMARY OF BENCHMARK MOLECULAR DATASETS WITH CATEGORIES, TASK COUNTS, AND DESCRIPTIONS.

| Datasets      | Category                   | Tasks | Description  |
|---------------|----------------------------|-------|--|
| BBBP          | physiology and toxicity    | 1     | a dataset with binary labels focusing on the barrier permeability of drugs which is a vital property for drugs targeting central nervous system. |
| BACE          | bioactivity and biophysics | 1     | a drug-target binding affinity dataset (binary label) for a set of inhibitors of human $\beta$ -secretase 1 (BACE-1)                             |
| ClinTox       | physiology and toxicity    | 2     | a dataset with two binary annotations where the first is to predict toxicity in clinical trials and the second is the FDA approval status.       |
| Tox21         | physiology and toxicity    | 12    | a dataset with binary labels of their toxic for 12 different targets including nuclear receptors and stress response pathways.                   |
| SIDER         | physiology and toxicity    | 27    | 1427 approved drugs with 27 different side effect groups and the task is to predict whether the drug is in the side effect group.                |
| ESOL          | physicochemical            | 1     | common organic small molecules with water solubility data (log solubility in mols per liter).  |
| FreeSolv      | physicochemical            | 1     | the hydration free energy of 642 molecules in water.   |
| Lipophilicity | physicochemical            | 1     | a dataset about octanol/water distribution coefficient (log $D$ at pH7.4) of compounds curated from ChEMBL database.                             |

**TABLE II. STATISTICS OF THE RYU AND DENG DATASETS.**

| <b>Dataset</b> | <b>Drugs</b> | <b>DDIs</b> | <b>Events</b> |
|----------------|--------------|-------------|---------------|
| Ryu            | 1,689        | 191,075     | 86            |
| Deng           | 572          | 74,528      | 65            |

**TABLE III. TOP TEN PREDICTED DRUGS THAT MAY INTERACT WITH QUINIDINE**

| <b>Index</b> | <b>Drug name</b>     | <b>Predicted interaction type</b>  | <b>Relevant evidence</b>  |
|--------------|----------------------|--|---|
| 1            | Mitotane             | The risk or severity of adverse effects can be increased when drug Quinidine is combined with drug Mitotane    | <a href="https://www.drugs.com/drug-interactions/dextromethorphan-quinidine-with-mitotane-3281-0-1643-0.html">https://www.drugs.com/drug-interactions/dextromethorphan-quinidine-with-mitotane-3281-0-1643-0.html</a> |
| 2            | Levodopa             | Drug Levodopa may decrease the cardiotoxic activities of drug Quinidine  | No evidence   |
| 3            | Halothane            | The metabolism of drug halothane can be decreased when combined with drug Quinidine                            | <a href="https://supp.ai/i/halothane-quinidine/C0018549-C0034414">https://supp.ai/i/halothane-quinidine/C0018549-C0034414</a>   |
| 4            | Isoflurane           | The metabolism of drug Isoflurane can be decreased when combined with drug Quinidine                           | <a href="https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308">https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308</a>   |
| 5            | Nandrolone decanoate | Drug Quinidine may decrease the antihypertensive activities of drug Nandrolone decanoate                       | No evidence   |
| 6            | Duloxetine           | Drug Quinidine may decrease the cardiotoxic activities of drug Duloxetine                                      | <a href="https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308">https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308</a>   |
| 7            | Desflurane           | The metabolism of drug Desflurane can be decreased when combined with drug Quinidine                           | <a href="https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308">https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308</a>   |
| 8            | Apalutamide          | The risk or severity of adverse effects can be increased when drug Quinidine is combined with drug Apalutamide | <a href="https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308">https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308</a>   |
| 9            | Acetohexamide        | Drug Quinidine may decrease the antihypertensive activities of drug Acetohexamide                              | <a href="https://www.drugs.com/drug-interactions/acetohexamide-with-quinidine-93-0-1981-0.html">https://www.drugs.com/drug-interactions/acetohexamide-with-quinidine-93-0-1981-0.html</a>                             |
| 10           | Dienogest            | Drug Quinidine may increase the hypotensive activities of drug Dienogest.                                      | <a href="https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308">https://reference.medscape.com/drug/quinaglute-quinidex-quinidine-342308</a>   |