The ADDI dataset used in our experiments is from the Twosides database, which was established by Tatonetti et al. that collected the reports of adverse drug reactions from FAERS caused by the administration of poly-pharmacy. We totally extract 25,495 adverse drug pairs from Twosides associated with 752 drugs and 1307 adverse interactions. This folder contains the detailed information of ADDI dataset, which consists of three files: **DrugSet.txt**, **AdverseInteractionSet.txt**, and **AdverseInteractionSetfromTWOSIDES.txt**. The details of the three files are provided in the following. We recommend to open these files by software Emeditor (available at https://www.emeditor.com/) that can better show the rows and columns of the files.

**DrugSet.txt** records the index of drugs (0-751), the drug identifier with prefix 'DB', and the drug name, in which the first column is the index of 752 drugs, the second column is the drug identifier with prefix 'DB', and the third column represents the drug name.

**AdverseInteractionSet.txt** provides the index of adverse interactions (0-1306), the identifiers of 1307 adverse interactions, and the name of 1307 adverse interactions. In particular, the first column is the indexes of all adverse intersections from 0-1306, the second column denotes the identifiers of 1307 adverse interactions from Twosides, and the third column is the names of 1307 adverse interactions.

**AdverseInteractionSetfromTWOSIDES.txt** is the adverse interaction dataset presented by the indexes of drugs from 0-751 and indexes of adverse interactions from 0-1306. To be specific, the first two columns are the drug indexes of an adverse drug pair (i.e., the first column in **DrugSet.txt**) and third column is the binary vector representing the adverse interaction vector caused by the adverse drug pair shown in the former two columns. **The dimension of the adverse interaction vector is the number of adverse interactions (i.e., 1307)**, where if the adverse drug pair can result in the *i*-th adverse interaction (the index of the adverse interaction corresponds to the first column in **AdverseInteractionSet.txt**), then the *i*-th element of the adverse interaction vector in the third column is 1; otherwise, the *i*-th element of the adverse interaction vector is 0. **Overall, this file consists of 25,495 rows,** indicating the ADDI dataset contains 25,495 adverse drug pairs. This file can be seen as the ground-truth adverse interactions among drugs that can be used for evaluating the results output by a prediction model.