

Title: Supplementary Data 1:

Description: results of cross-validation experiment on training data for each of four machine learning models on each of 13 drugs.

Title: Supplementary Data 2:

Description: top 1% of highest saliency positions for each drug detected by the MD-CNN model

Title: Supplementary Data 3:

Description: top 1% of highest saliency positions for each drug detected by the SD-CNN model