Supplementary Files

**Supplementary File 1**: Drug-domain interactions.txt

The drug-domain interactions, where the identifiers of drugs are DrugBank identifiers and identifiers of domains are Pfam identifiers. The first column lists drugs, the second column lists domains, and the third lists the probability of interaction between corresponding drugs and domains.

**Supplementary File 2**: Modules\_drug.xls

The detailed module information with corresponding memberships, where the first column lists modules and the second lists drugs with associated ATC codes located in corresponding modules, and the identifiers of drugs are DrugBank identifiers.

**Supplementary File 3**: Drug-target interactions.txt

Predicted drug-protein interactions based on drug-domain interactions. The first column lists drugs with DrugBank identifiers, the second column lists proteins with gene symbols and the third is the probability of interaction between corresponding drug and protein.

**Supplementary Figure 1**: S\_Fig1.tif

The domain compositions of all drug target proteins (Supplementary Fig.1 A) and our predicted ones (Supplementary Fig.1 B).