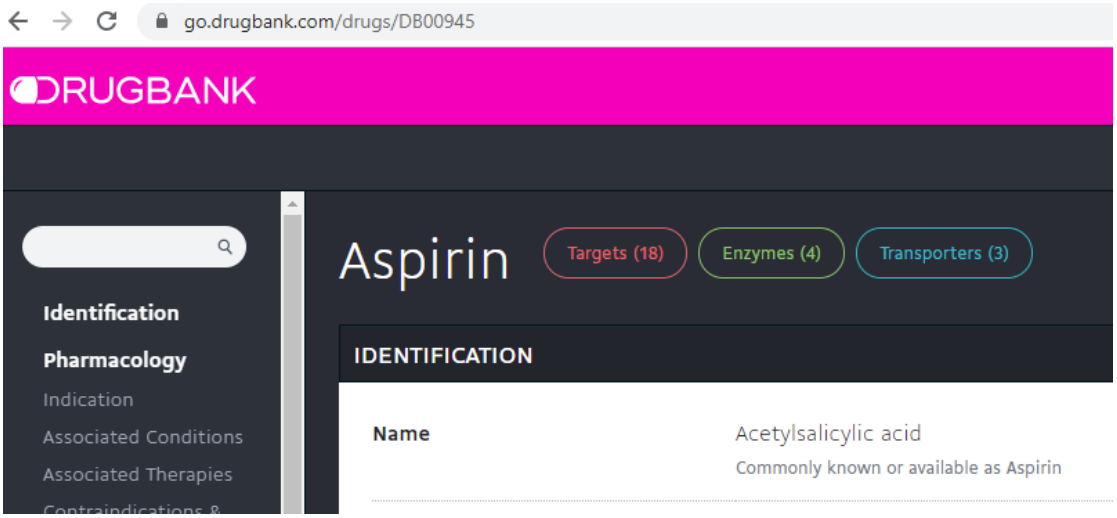
How to obtain the document and DTI triplets from DrugBank?

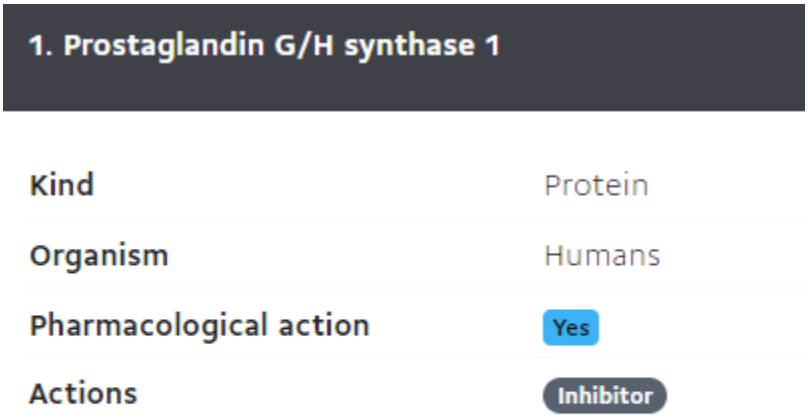
Take “Aspirin” as an example.

S-1: On DrugBank, we input “Aspirin and get



S-2: Press the Botton “Targets (18)”, we will see the targets of Aspirin.

We show an example here:



We can see that the target name is “Prostaglandin G/H synthase 1”, and the interaction is “inhibitor”. Therefore, we obtain a triplet < Aspirin , Prostaglandin G/H synthase 1, inhibitor >

S-3: For references, the related work on target “Prostaglandin G/H synthase 1” include:

1. Flipo RM: [Are the NSAIDs able to compromising the cardio-preventive efficacy of aspirin?]. Presse Med. 2006 Sep;35(9 Spec No 1):1S53-60. [PubMed:17078596]
2. Schwartz KA: Aspirin resistance: a review of diagnostic methodology, mechanisms, and clinical utility. Adv Clin Chem. 2006;42:81-110. [PubMed:17131625]
3. Birnbaum Y, Ye Y, Lin Y, Freeberg SY, Huang MH, Perez-Polo JR, Uretsky BF: Aspirin augments 15-epi-lipoxin A4 production by lipopolysaccharide, but blocks the pioglitazone and atorvastatin induction of 15-epi-lipoxin A4 in the rat heart. Prostaglandins Other Lipid Mediat. 2007 Feb;83(1-2):89-98. Epub 2006 Nov 7. [PubMed:17259075]
4. Guthikonda S, Lev EI, Patel R, DeLao T, Bergeron AL, Dong JF, Kleiman NS: Reticulated platelets and uninhibited COX-1 and COX-2 decrease the antiplatelet effects of aspirin. J Thromb Haemost. 2007 Mar;5(3):490-6. [PubMed:17319904]
5. Durlaza FDA label [File]

For those with [PubMed:id] , we can download the abstracts from the following two websites:
https://ftp.ncbi.nlm.nih.gov/pubmed/baseline
https://ftp.ncbi.nlm.nih.gov/pubmed/updatefiles/

Therefore, we successfully find documents for the aforementioned DTI triplet.

DrugBank provides a xml file, that contains all information of its website. We parse the XML files to obtain the above information.

How to obtain the document and DTI triplets from TTD?

S-1: go to website http://db.idrblab.net/ttd/sites/default/files/ttd_database/P1-07-Drug-TargetMapping.xlsx, download the excel form.

S-2: we can directly parse the drug, target, interaction and pubmed id from it.