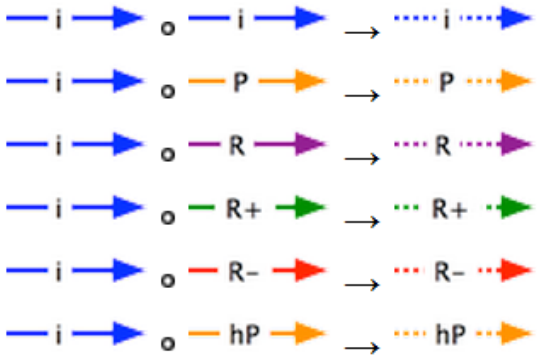
Functional Therapeutics Classification

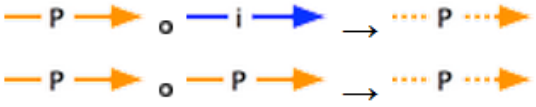
FTC

Go Relations

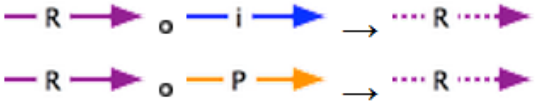
is a ∘ …



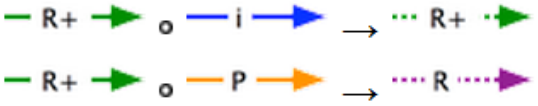
part of ∘ …



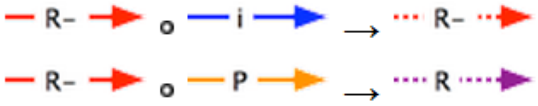
regulates ∘ …

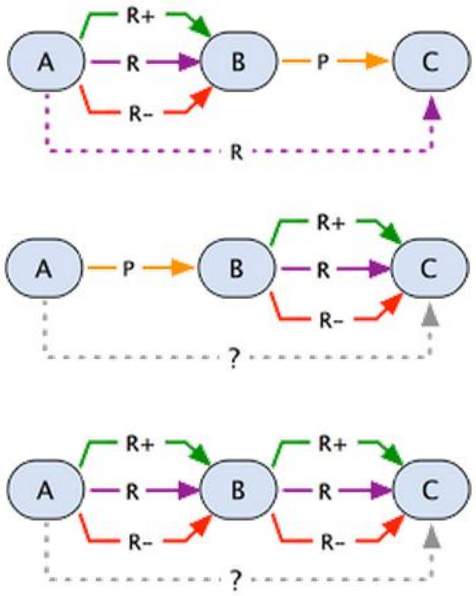


positively regulates ∘ …



negatively regulates ∘ …





The regulation of the mechanism is assumed to be un-uncoupled to the mechanism, in other words: The mechanism can happen without the regulation

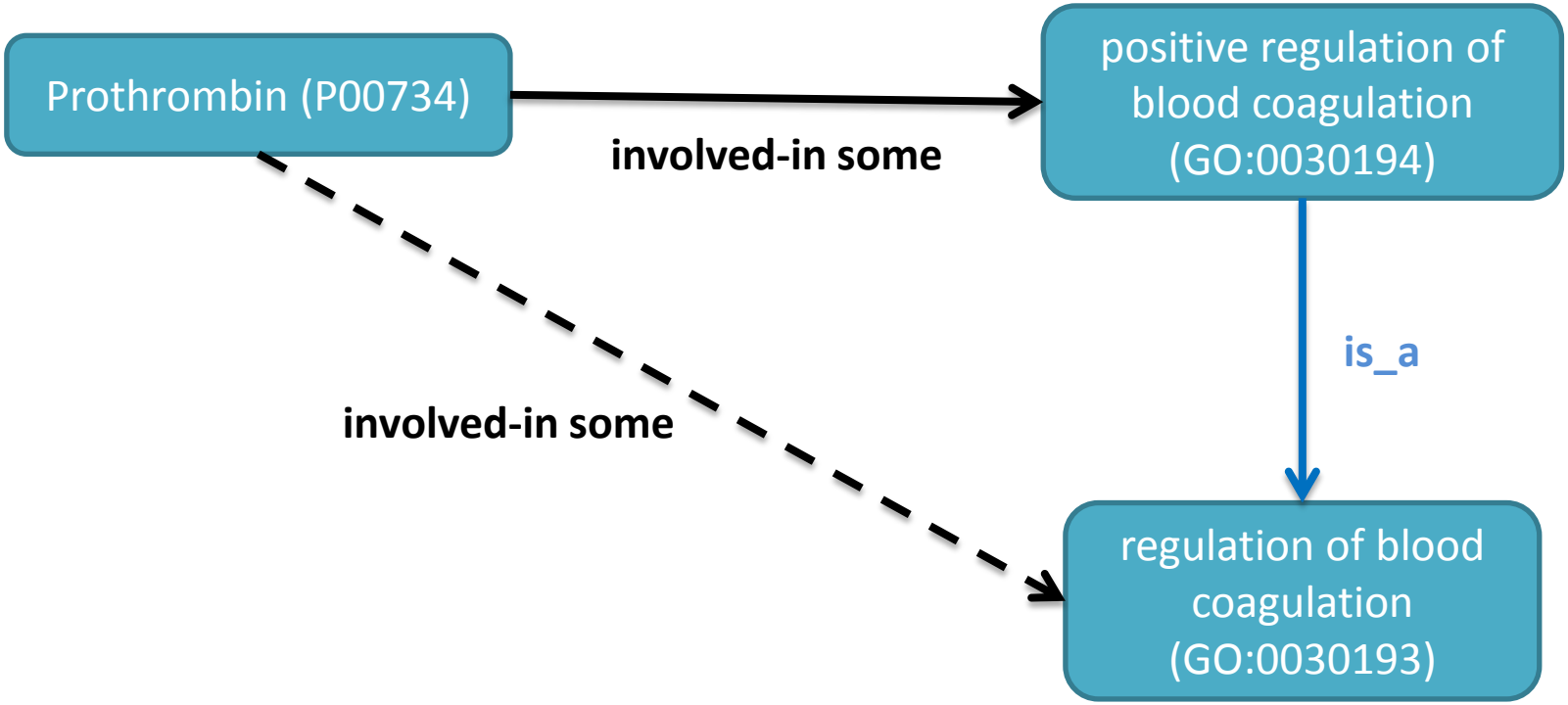
ftc:involved-in

- Range: Gene products (Activity)
- Domain: Bio-Process
- Comment: Coming from GOA, annotation of a gene product with a bio-process

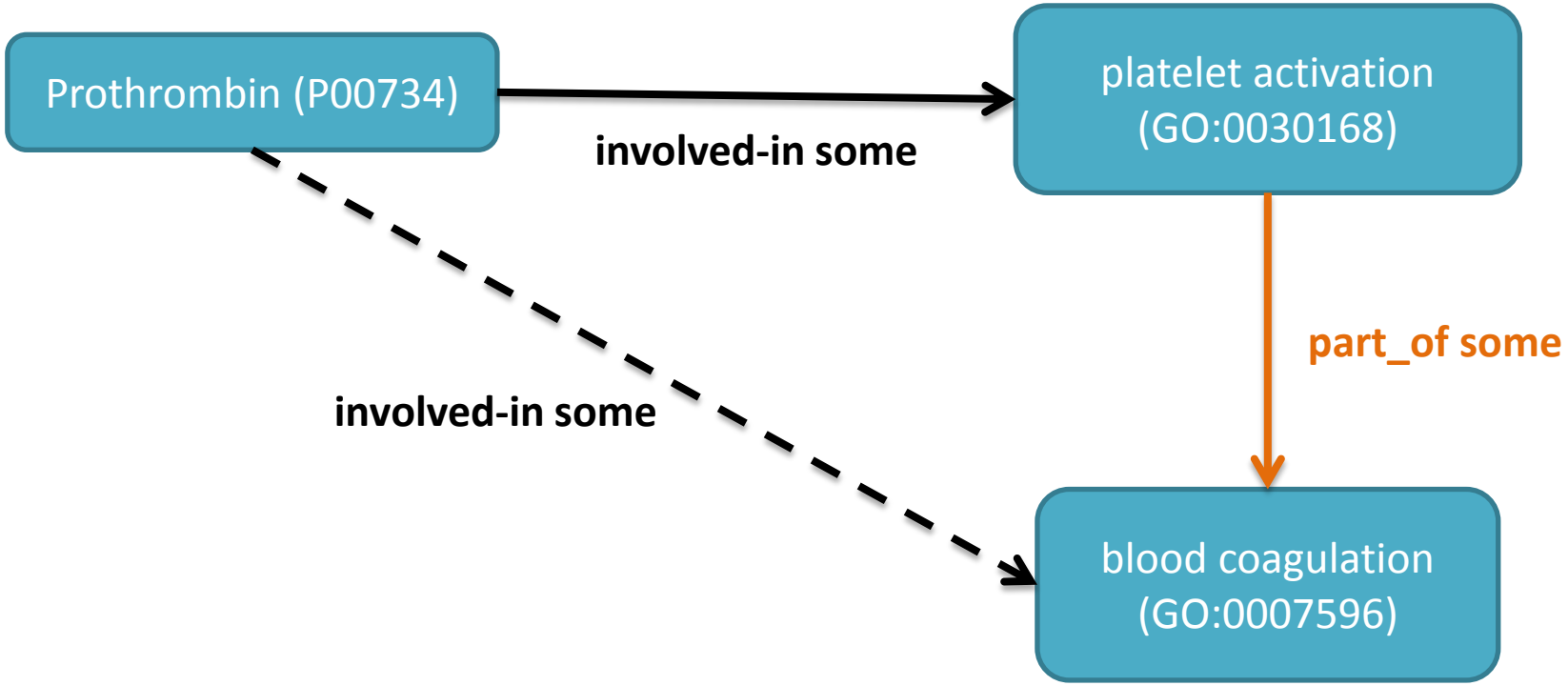
- Chain Properties:
- ftc:involved-in **o** ro:is_a → ftc:involved-in
- (ro:is_a **o** ftc:involved-in → ftc:involved-in)
- ftc:involved-in **o** ro:part-of → ftc:involved-in
- ftc:involved-in **o** ro:regulates → ???

- Other combinations are impossible due to range and domain restrictions.

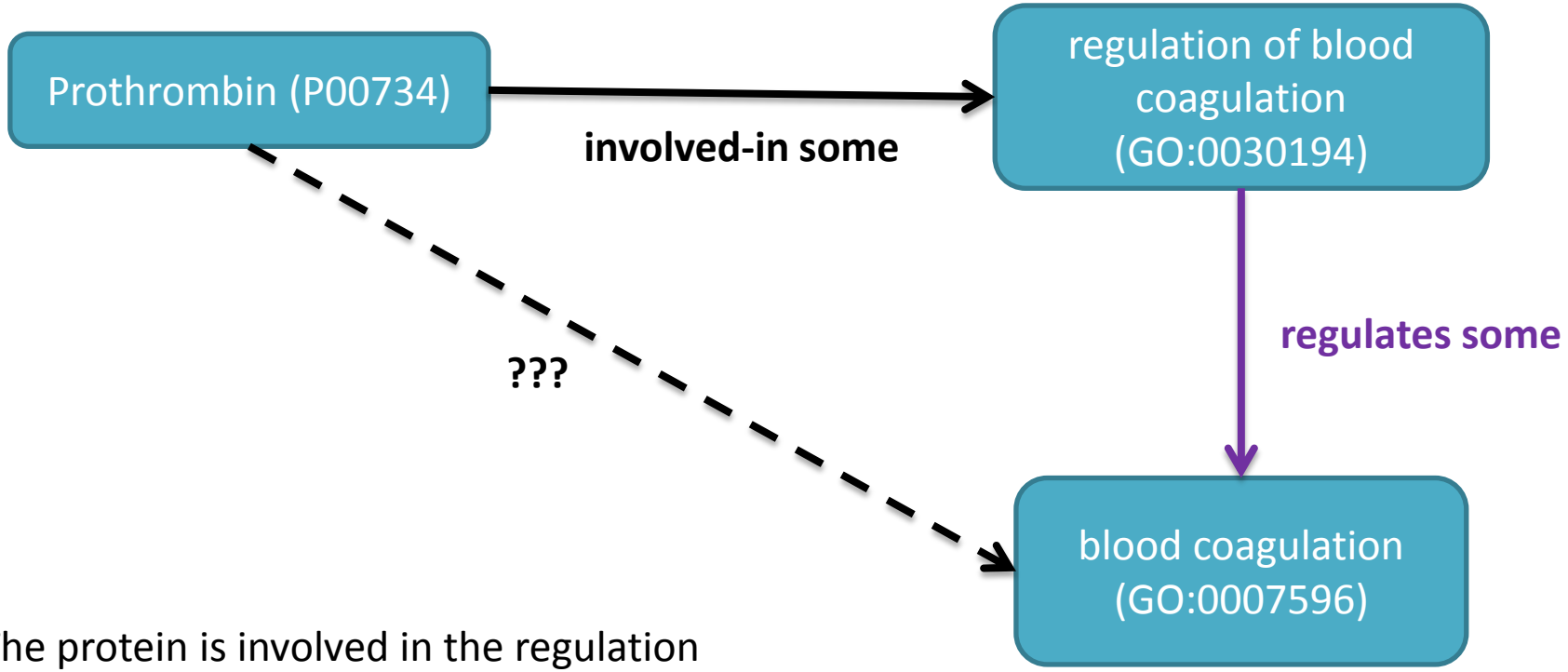
ftc:involved-in **o** ro:is_a → ftc:involved-in



ftc:involved-in **o** ro:part-of → ftc:involved-in



ftc:involved-in **o** ro:regulates → ???



The protein is involved in the regulation process, not the process itself. A bit ambiguous, but inline with GO.

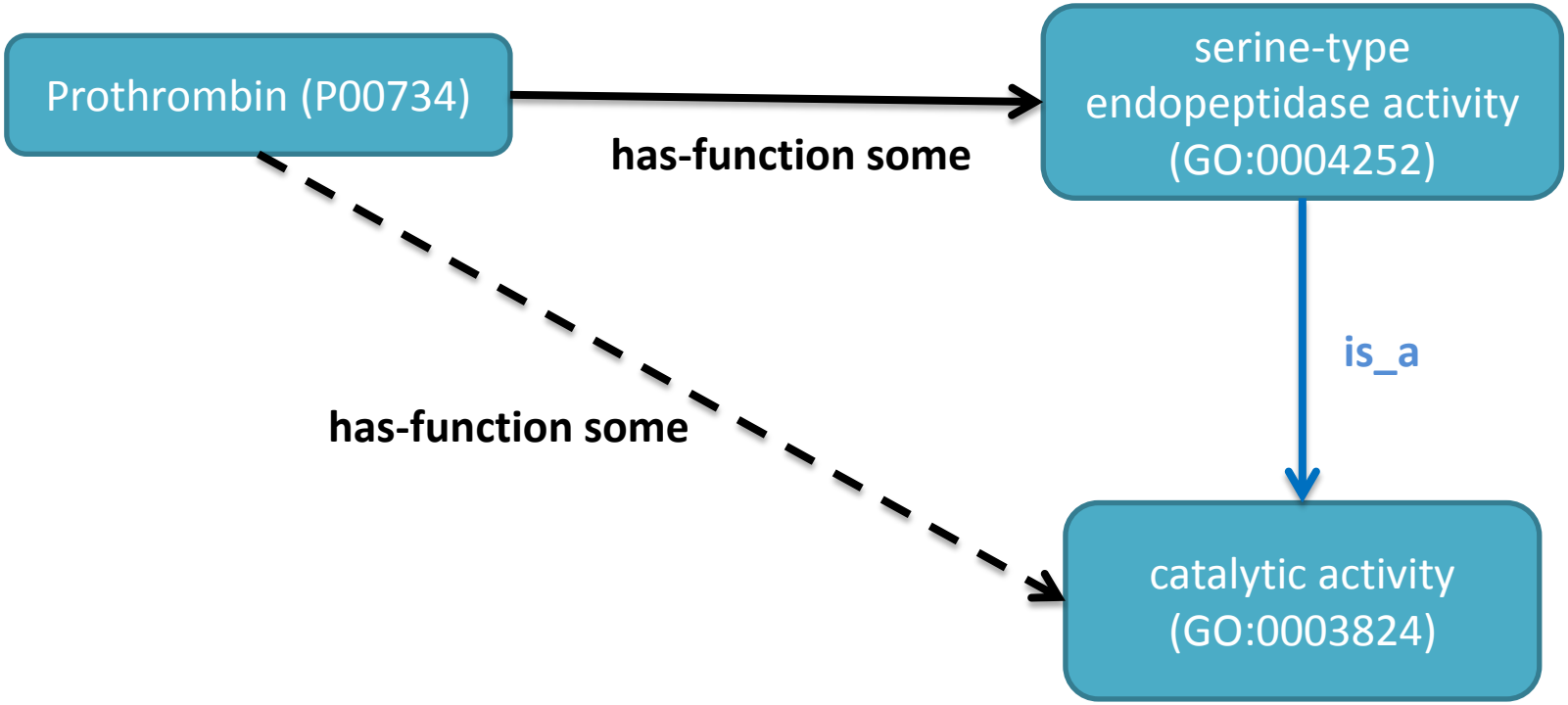
ftc:has-function

- Range: Gene products (Activity)
- Domain: Molecular Function
- Comment: Coming from GOA, annotation of a gene product with a function.

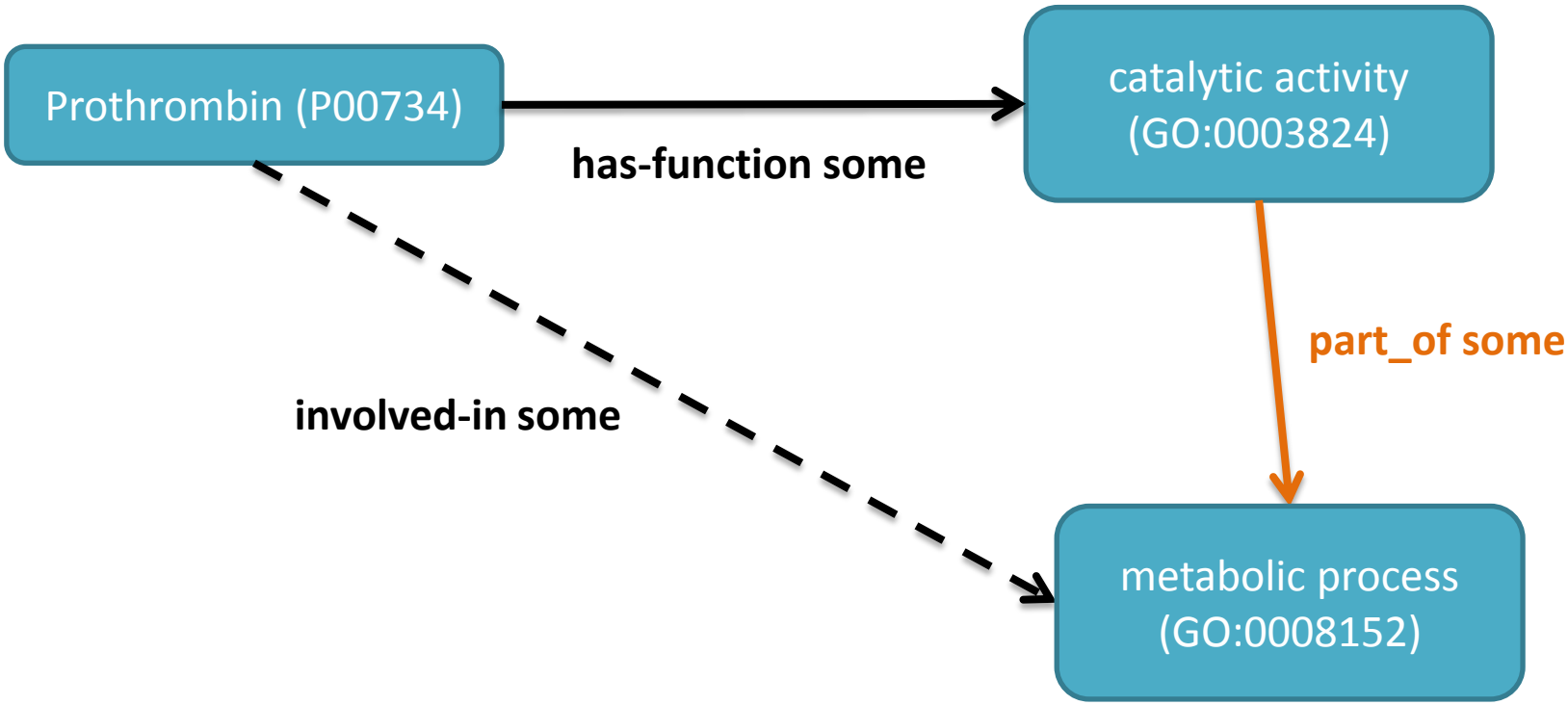
- Chain Properties:
- ftc:has-function **o** ro:is_a → ftc:has-function
- (ro:is_a **o** ftc:has-function → ftc:has-function)
- ftc:has-function **o** ro:part-of → ftc:involved-in

- Other combinations are impossible due to range and domain restrictions.

ftc:has-function **o** ro:is_a → ftc:has-function



ftc:has-function **o** ro:part-of → ftc:involved-in



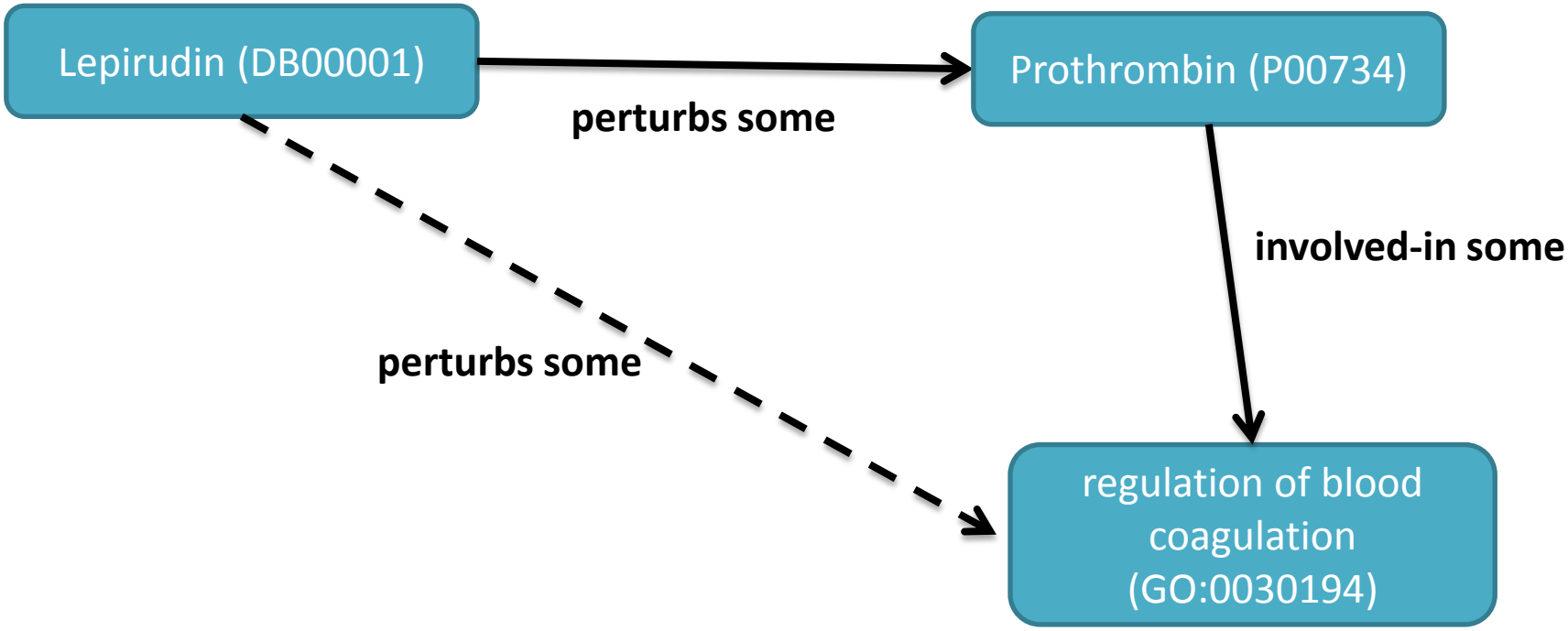
ftc:perturbs

- Range: Chemical Compounds (Activity)
- Domain: Gene Product (Activity)
- Comment: Coming from a chemical (drug), reflects the action on the gene product.

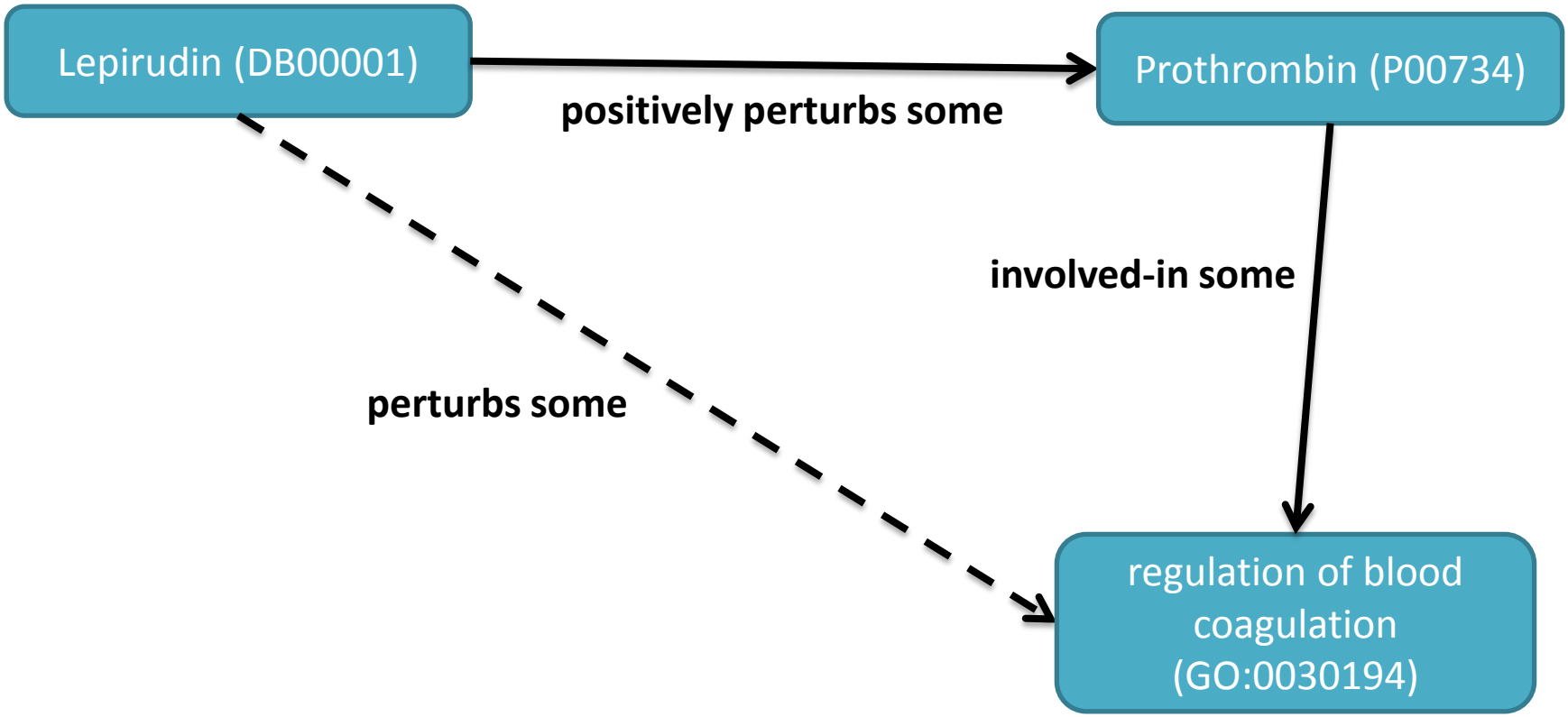
- Chain Properties:
- (ftc:pertubs **o** ro:is_a → ftc:pertubs)
- (ro:is_a **o** ftc:pertubs → ftc:pertubs)
- ftc:pertubs **o** ro:involved-in → ftc:pertubs
- ftc:positively-pertubs **o** ro:involved-in → ftc:pertubs
- ftc:negatively-pertubs **o** ro:involved-in → ftc:pertubs
- ftc:pertubs **o** ro:part-of → ftc:pertubs
- ftc:pertubs **o** ro:regulates → ???

- Other combinations are impossible due to range and domain restrictions.

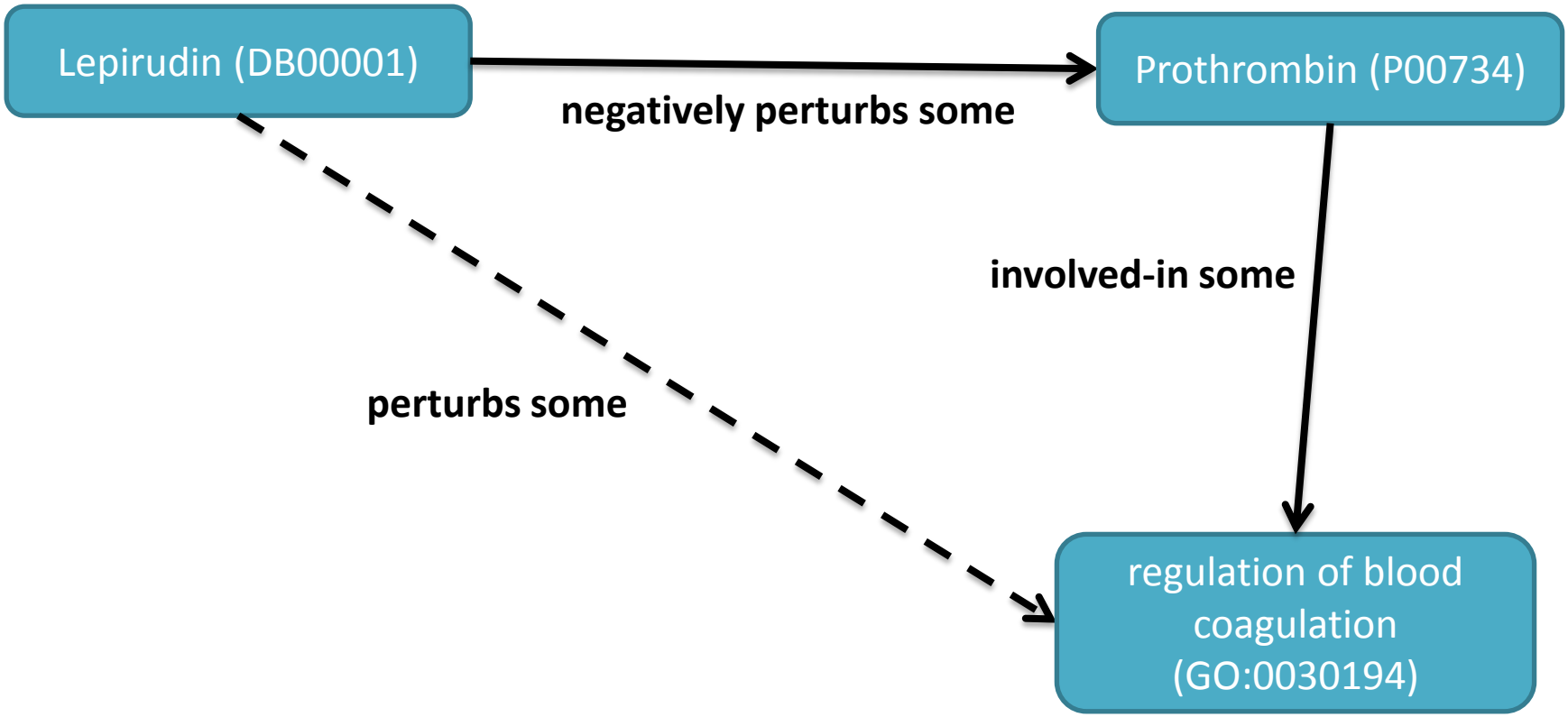
ftc:pertubs **o** ro:involved-in → ftc:pertubs



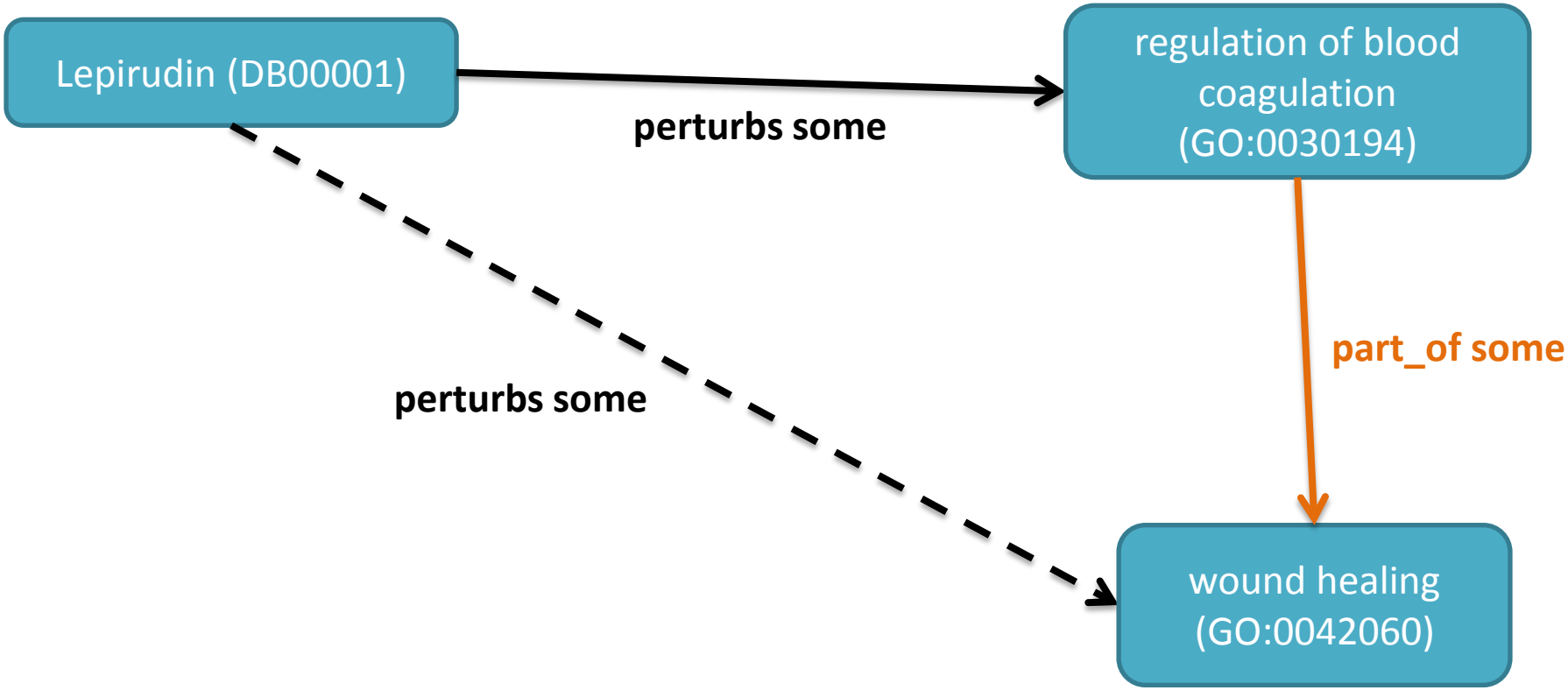
ftc:positively-pertubs **o** ro:involved-in → ftc:pertubs



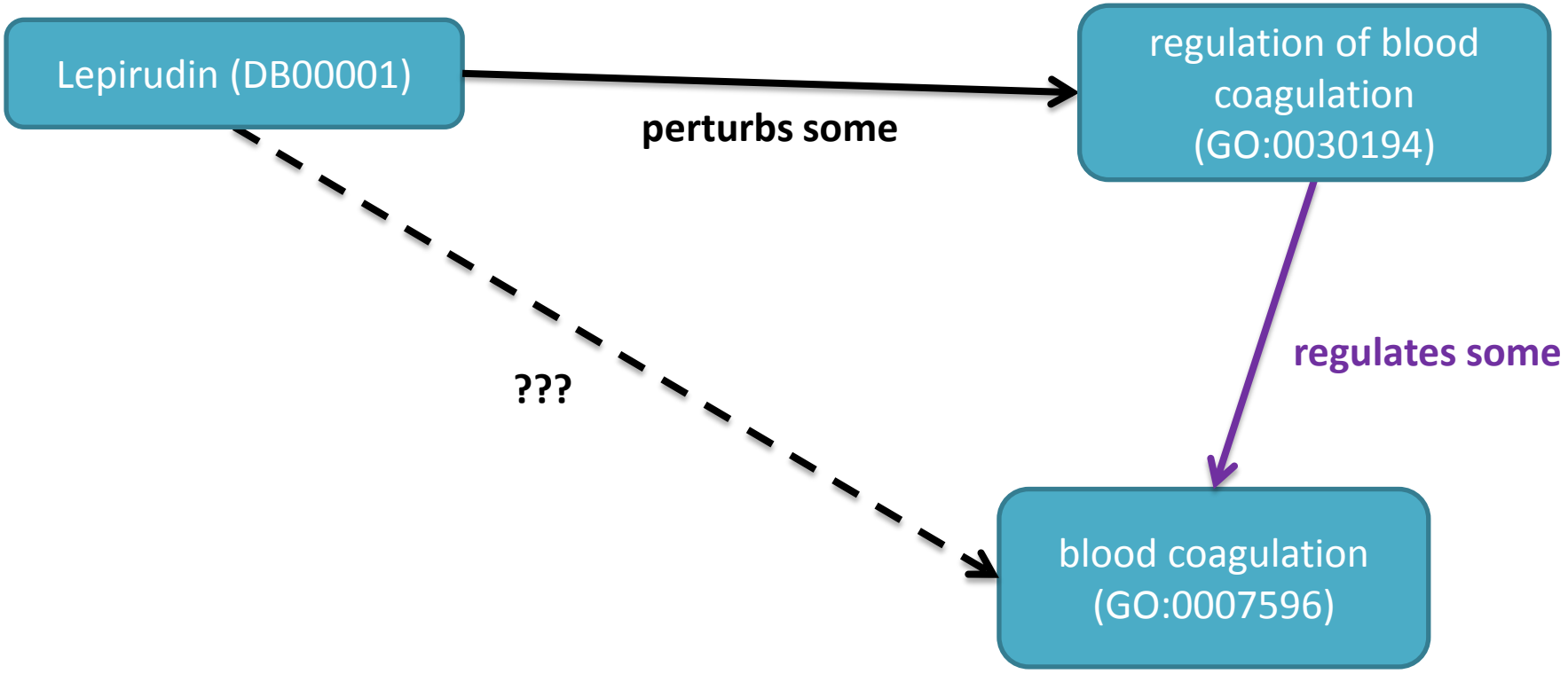
ftc:negatively-pertubs **o** ro:involved-in → ftc:pertubs



ftc:pertubs **o** ro:part-of → ftc:pertubs



ftc:pertubs **o** ro:regulates → ???



ftc:Agent

ftc:Anti-Biological-Process-Agent:

Drug and (positively-perturbs some (Protein and (involved-in some negative_regulation_of_biological_process)))

Drug and (negatively-perturbs some (Protein and (involved-in some positive_regulation_of_biological_process)))

ftc:Pro-Biological-Process-Agent:

Drug and (positively-perturbs some (Protein and (involved-in some positive_regulation_of_biological_process)))

Drug and (negatively-perturbs some (Protein and (involved-in some negative_regulation_of_biological_process)))

ftc:Therapeutic_Compound

- Drugs from DrugBank are subclasses of that class

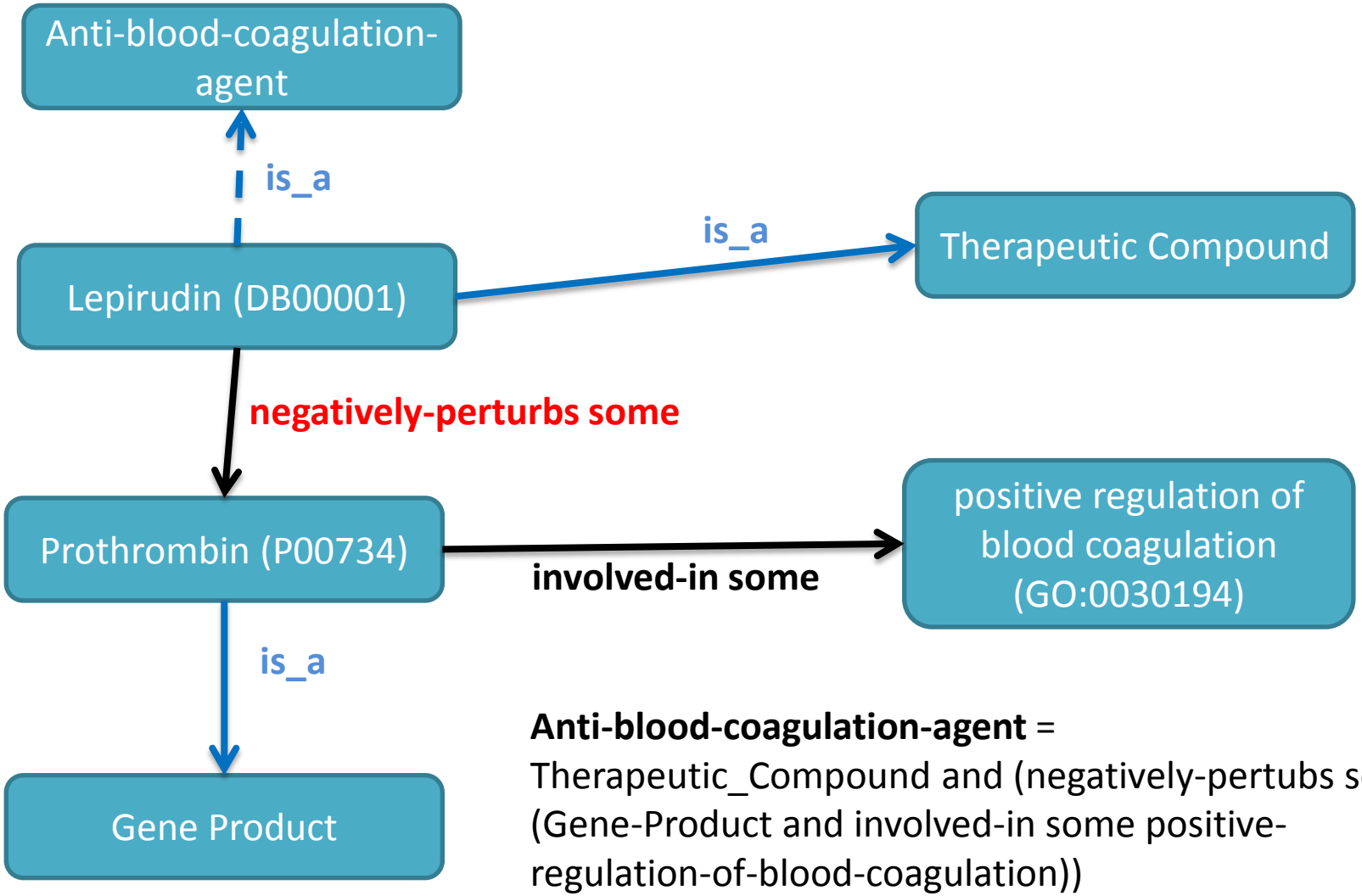
ftc:Gene_Product

- Gene products (proteins) are sub-classes of this class
- What about non gene-products that are targets of drugs?

Classes from GO

- Go:Biological_Process and go:molecular_function are also top level

Anti/Pro Patterns



Anti-blood-coagulation-agent = Therapeutic_Compound and (negatively-pertubs some (Gene-Product and involved-in some positive-regulation-of-blood-coagulation))

Problems

- Proteins with multiple functions (multiple domains) that are the target of the drug. Only part of the functions are perturbed, not everything.
- At the moment deal only with human proteins
- What about other organisms, like bacteria, etc…?

Pseudo-Code

```
Foreach(drug){
        Foreach(target){
                foreach(getAllAnnotations()){
                        if(annot is BP r+/r- regulating){
                                create class
                        }
                        if(annot is MF){
                                create class
                        }
                }
        }
}
```