



An Ontology for formal representation of Drug-Drug Interaction Knowledge

María Herrero-Zazo, Isabel Segura-Bedmar, Paloma Martínez
Computer Science Department, Universidad Carlos III de Madrid, Spain
{mhzazo, isegura, pmf}@inf.uc3m.es



Motivation:

- A drug-drug interaction (DDI) occurs when one drug influences the level or activity of another drug.
- Drug Interaction databases are rarely complete => Medical literature is the most effective source for the detection of drug interactions.
- The process that leads to DDI may involve pharmacokinetics (ADME) and pharmacodynamic processes. Therefore, the biological mechanisms underlying DDIs include interactions with metabolic enzymes, protein transports and drug targets.
- The formal representation of this knowledge can be useful for: data annotation tasks, drug discovery, *in silico* prediction of DDIs and early detection in clinical practice, improvement of Clinical Decision Support Systems, development of signal detection methods in Pharmacovigilance, integration in Electronic Medical Records, etc.



The DDI Corpus

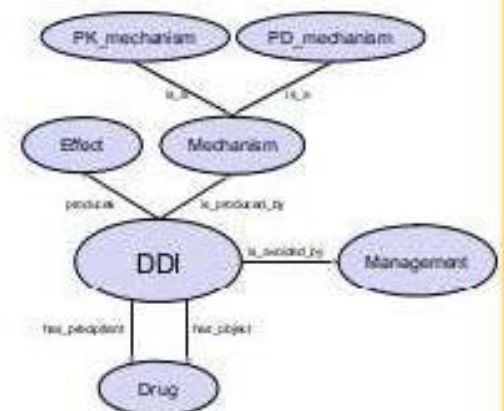
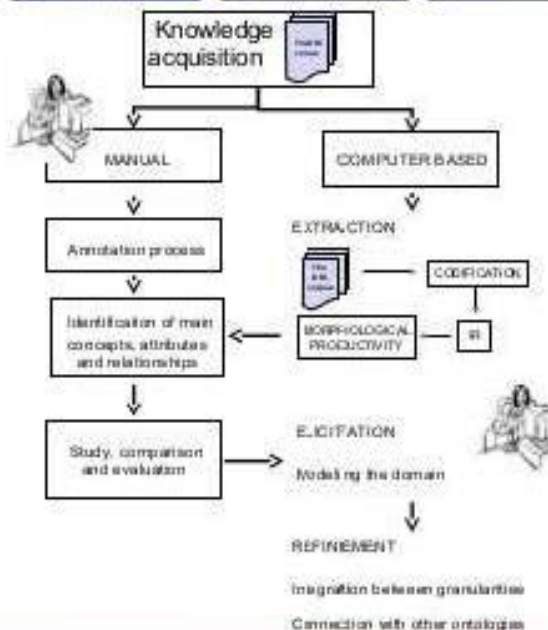
- The largest corpus for DDI Extraction
- Two different types of documents: DrugBank drug interaction fields and MedLine abstracts.
- Annotation of different types of pharmacological substances and PK and PD DDIs.
- Manually annotated by two annotators relying in specific annotation guidelines.
- Measurement of Inter-Annotator Agreement (IAA).
- Publicly available.
- The DDI Corpus is being used in the DDI Extraction 2013 task, for the recognition of drug names and extraction of drug-drug interactions in biomedical literature.

		Total
Documents	DrugBank	792
	MedLine	233
Sentences	DrugBank	6,795
	MedLine	2,147
Entities		18,502
DDIs Relationships		5,028



The Drug-Drug Interactions Ontology

1st Prototype Life Cycle



A preliminary Semantic Network Representing DDI Knowledge Structure

ACKNOWLEDGMENTS:

This work was supported by the Regional Government of Madrid under the Research Network MA2VICMR [S2009/TIC-1542] and by the Spanish Ministry of Education under the project MULTIMEDICA [TIN2010-20644-C03-01]

We thank the team at the Humboldt-Universität zu Berlin for making available a visualization of the DDI corpus using Stav:

<http://http://corpora.informatik.hu-berlin.de/>

<https://github.com/TsujiiLaboratory/stav>