Drug-drug interactions (DDIs) form a significant risk group for adverse effects associated with pharmaceutical treatment. These interactions are often reported in the literature, however, they are sparsely represented in machine-readable resources, such as online databases, thesauri or ontologies. Although previous research works attempted a formal representation of this domain, none of them provided a comprehensive conceptualization of DDIs. In addition to this, these ontologies were evaluated in one of two main applications: natural language processing (NLP) or inference of DDIs based on their pharmacological mechanisms, but never used in more than one task. In this scenario, we created DINTO, an ontology that describes and categorizes DDIs and all their possible mechanisms. This ontology reuses information from other ontologies − such as pharmacological substances from the ChEBI ontology or adverse drug reactions (ADR) from the Ontology of Adverse Events (OAE) − and databases − including drug-protein relationships from DrugBank or ADR from SIDER. DDI mechanisms, or the pharmacological process leading to the occurrence of a DDI, are represented as Semantic Web Rule Language (SWRL) rules, including different types of pharmacokinetic and pharmacodynamics DDIs. Therefore, this is the first ontology providing a detailed representation of all the most important types of DDI mechanisms. The final ontology consists in more than 28,000 classes (including 8,000 drugs and 11,500 DDIs), 73 object properties and 17 data properties. It has been used in two different applications: NLP and inference of DDIs. The ontology was used for both tasks − named entity recognition and relation extraction – and the SWRL rules were combined with the drug-target and drug-ADR relations represented in DINTO to predict DDIs and their mechanisms in a large scale.

In future work, we plan to extent the content of the ontology including drug-related information crucial for DDIs – such as drug bioactivity data, therapeutic index of drugs, or physicochemical properties – as well as updated and integrated information of drug-protein relations and ADRs. However, these achieving these goals requires facing challenges such as large data integration, updating and maintenance of large ontologies, which might bring an interesting discussion topic in this session.