Relation Extraction from Biomedical Literature on Pharmacokinetic Natural Product-Drug Interactions

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INTRODUCTION

BACKGROUND

Co-consumption of natural products such as green tea with drugs can lead to pharmacokinetic natural product-drug interactions (NPDIs).

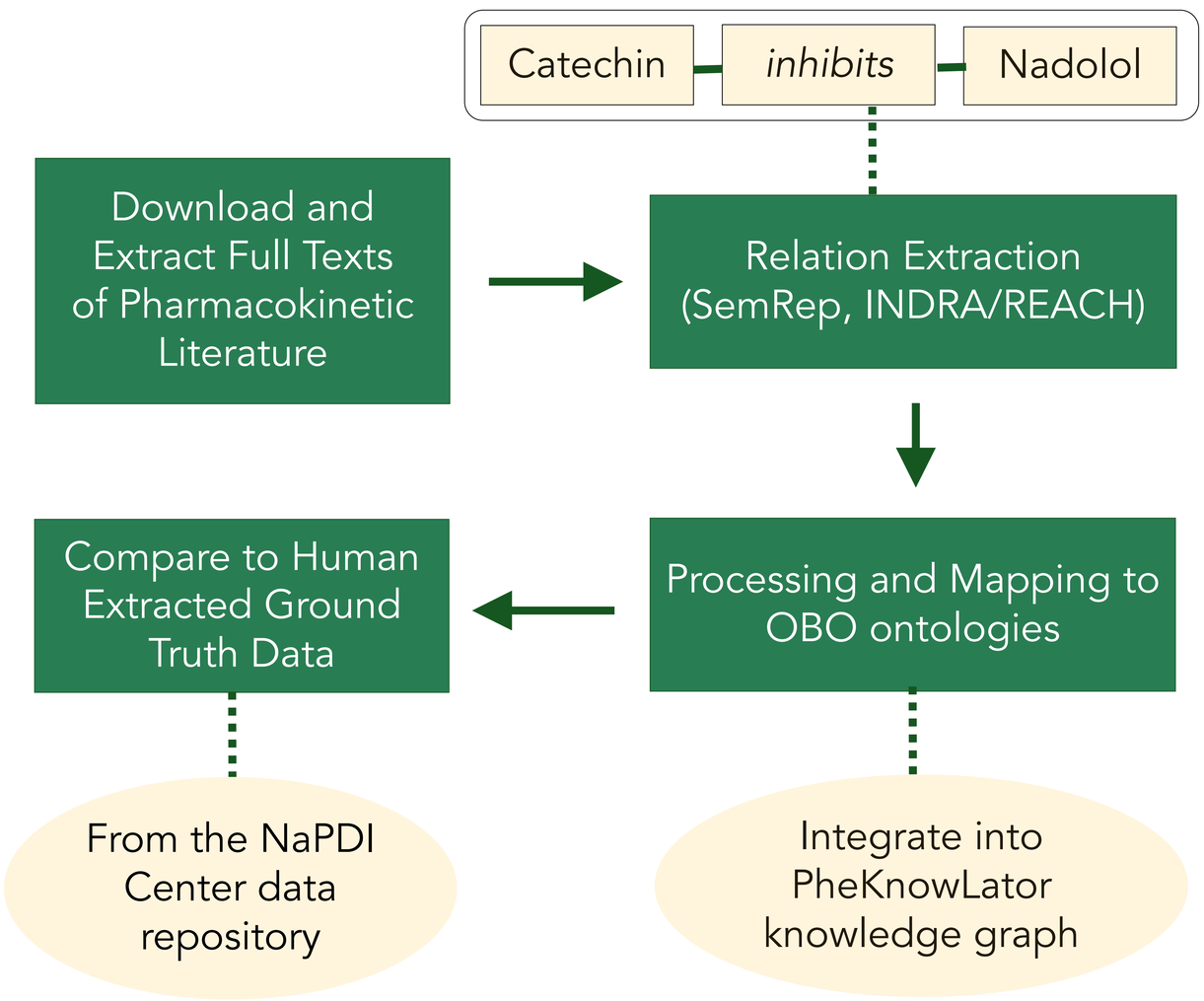
MOTIVATION

We need to understand the mechanism of NPDIs to prevent unwanted drug response and promote safe use of natural products. Scientific literature *(in vitro* and clinical*)* contains insights about these mechanisms.

OBJECTIVE

We extract predications (*subject-predicate-object* triples) from full texts of articles focused on green tea-related pharmacokinetic interactions from 2 relation extraction systems and compare with human extracted data.

METHODS

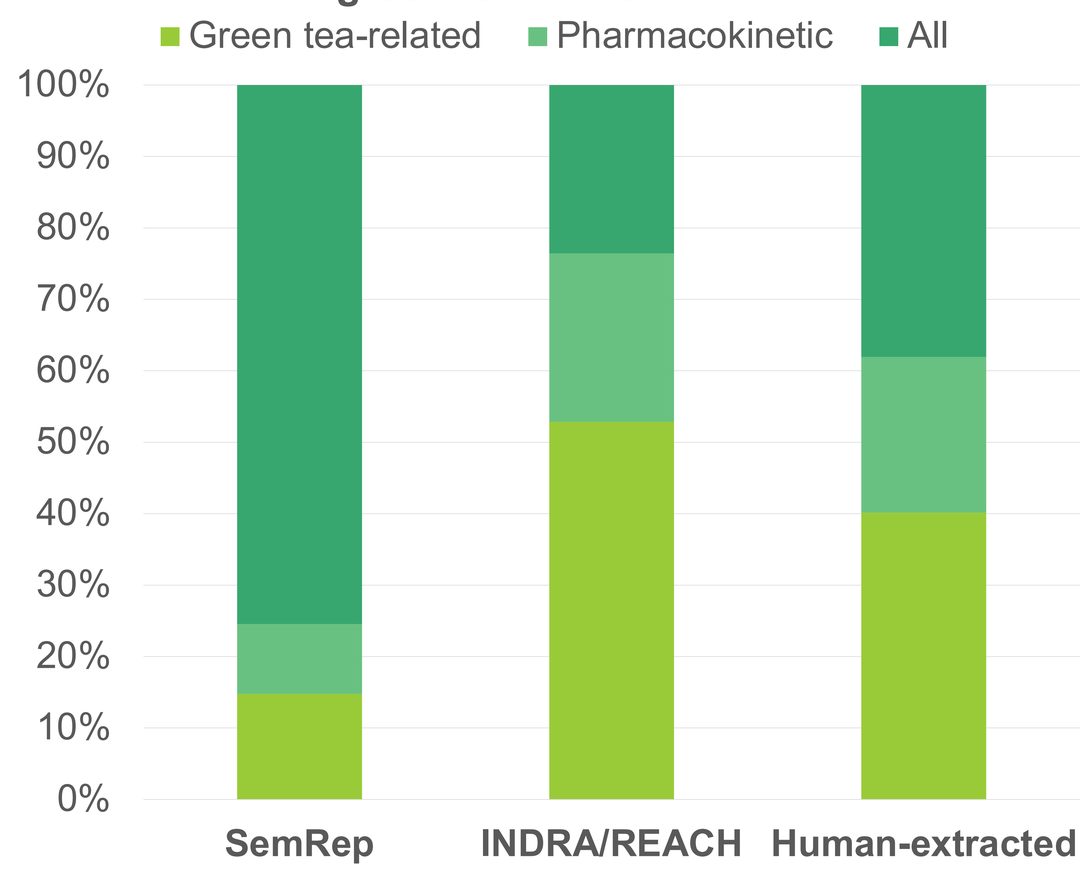


INDRA: Integrated Network and Dynamic Reasoning Assembler
REACH: Reading and Assembling Contextual and Holistic Mechanisms from Text
OBO: Open Biological and Biomedical Ontology

Kilicoglu H, Rosemblat G, Fiszman M, Shin D. Broad-coverage biomedical relation extraction with SemRep. BMC Bioinformatics. 2020 May 14;21(1):188.
Gyori BM, Bachman JA, Subramanian K, Muhlich JL, Galescu L, Sorger PK. From word models to executable models of signaling networks using automated assembly. Mol Syst Biol. 2017 Nov 1;13(11):954.
Valenzuela-Escárcega MA, Babur Ö, Hahn-Powell G, Bell D, Hicks T, Noriega-Atala E, et al. Large-scale automated machine reading discovers new cancer-driving mechanisms. Database J Biol Databases Curation. 2018 01;2018.

RESULTS

Recall (SemRep) = 0.31
Recall (INDRA/REACH) = 0.20
Recall (Combined) = 0.42



Pharmacokinetic Predicate	SemRep	INDRA/ REACH	Human Extracted
INHIBITS	38	79	80
INTERACTS WITH	54	0	46
ACTIVATES/STIMULATES	13	40	0
SUBSTRATE OF*	0	0	23
OTHER	88	4	30
TOTAL	193	123	179

Table 1: Number of pharmacokinetic predications extracted by predicate type from SemRep and INDRA/REACH

CONCLUSION

Semantic relation extraction can find associations between biomedical entities to inform scientists of prior work.

Evaluation with full texts shows both advantages and limitations for discovering mechanistic hypotheses about NPDIs.

For more details:
https://github.com/sanyabt/napdi-kg, https://repo.napdi.org/

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