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RESEARCH ARTICLE

Purdue Ontology for Pharmaceutical Engineering: Part II. Applications

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Abstract The multiple steps in pharmaceutical product development generate a large amount of diverse information in various formats, which hinders efficient decision-making. A major component of the solution is a common information model for the domain. Ontologies were found to meet this need as described in Part I of this two-part paper. In Part II, we describe two applications of Purdue Ontology for Pharmaceutical Engineering. The first application deals with the prediction of degradation reactions through incorporation of molecular structure and environmental information captured in the ontologies. The second application is one that analyzes experiments to identify differences in experimental implementation.

Keywords Ontology · Informatics · Reaction prediction · Experiment analysis

Introduction

A staggering volume and variety of information, ranging from raw experimental data to lab reports to complex mathematical models needs to be stored, accessed, validated, manipulated, managed, and used for pharmaceutical drug development. This information is often in different formats, uses different software solutions, and difficult to integrate. A common, explicit, and platform-independent vocabulary that is both machine accessible and human usable is needed to streamline the flow of information and knowledge generation. This can be done using ontologies (descriptions of a domain through its concepts and relations between those concepts [1]). The Purdue Ontology for Pharmaceutical Engineering (POPE) was developed to address the informatics challenge described above [2]. POPE includes several components as shown in Fig. 1. The expert knowledge is modeled in the form of guidelines in the ontological infrastructure. A guideline models procedural knowledge, which consists of decision logic, information look-up, evaluation of decision variables, and provision of recommendations. POPE also describes mathematical knowledge, which consists of the mathematical equations as well as the underlying assumptions on the phenomenon.

Further details on the guideline ontologies and mathematical knowledge ontologies are provided elsewhere [2, 3]. The information ontologies shown in Fig. 1 have several components. These include the Purdue Ontology for Material Entities (POME) which describes phases, substances, and compositions; Purdue Ontology for Molecular Structure (POMS) which describes molecular structures; Purdue Ontology for Reaction Engineering (PORE) which describes chemical and physical reactions; Purdue Ontology for Material Properties (POMP) which describes physical and chemical properties; Purdue Ontology for Description of Experiments (PODE) which describes experiments, procedures, and settings; Purdue Ontology for Characterization of Equipment, Purdue Ontology for Description of Unit Processes and the Purdue Ontology for Value Description. Further description of these ontologies is given in Part I of this paper [4]. Once developed, these ontologies can be populated with information and data from relational data-

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