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Esta revista é (e sempre foi) eletrônica para ajudar a proteger o meio ambiente, mas, caso deseje imprimir esse artigo, saiba que ele foi editorado com uma fonte mais ecológica, a *Eco Sans*, que gasta menos tinta.

*This journal is (and has always been) electronic in order to be more environmentally friendly. Now, it is desktop edited in a single column to be easier to read on the screen. However, if you wish to print this paper, be aware that it uses Eco Sans, a printing font that reduces the amount of required ink.*

# UMA ONTOLOGIA DE AGRAVOS CAUSADOS PELO USO INADEQUADO DE AGROTÓXICOS

## AN ONTOLOGY OF DISEASES CAUSED BY IMPROPER USE OF PESTICIDES

(artigo submetido em junho de 2014)

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### ABSTRACT

The indiscriminate use of pesticides is one of the main factors contributing towards the chemical contamination of human beings, causing various types of intoxications. However, accessing information about pesticides and the consequences of their use, has proven difficult. Therefore, the present paper describes the development of an ontology which has the purpose of structuring knowledge in the field of health, focusing on diseases caused by the improper and indiscriminate use of pesticides. The ontology developed, called OntoTox was based on documents with a pesticide classification and the intoxication caused by their use. OntoTox was constructed according to the Methontology method, as well as some steps of the 101 method and implemented in the Protégé environment. This ontology was evaluated by the Data-Driven method as well as the response to questionnaires administered to experts in the fields of health and agriculture. They considered it a valid source of knowledge in aiding the diagnosis of poisoning and health problems related to the use of pesticides. This ontology can be used in providing aid to victims of poisoning and in research involving pesticides and poisoning.

Key-words: ontology; diseases; pesticides; knowledge; intoxications.

### RESUMO

O uso indiscriminado de agrotóxicos é um dos principais fatores que contribuem para a contaminação química dos seres humanos, causando vários tipos de intoxicações. No entanto, o acesso a informações sobre os pesticidas e as consequências de seu uso tem sido difícil. Portanto, o presente artigo descreve o desenvolvimento de uma ontologia que tem a finalidade de estruturar conhecimentos no campo da saúde, incidindo sobre doenças causadas pelo uso indevido e indiscriminado de pesticidas. A ontologia desenvolvida, chamada OntoTox, foi baseada em documentos com classificação de pesticidas e da intoxicação causada pelo seu uso. OntoTox foi construída de acordo com o método Methontology, bem como algumas fases do método 101 e implementada no ambiente Protégé. Esta ontologia foi avaliada pelo método orientado a dados, bem como a resposta a questionários aplicados com especialistas nas áreas de saúde e agricultura. Eles a consideraram uma fonte válida de conhecimento para ajudar no diagnóstico de problemas de intoxicação e de saúde relacionados ao uso de pesticidas. Esta ontologia pode ser utilizada na prestação de ajuda às vítimas de envenenamento e na pesquisa com agrotóxicos e intoxicação.

**Palavras chaves:** ontologia; doenças; pesticidas; conhecimento; intoxicações.

## 1 INTRODUCTION

The development of pesticide related diseases around the globe has encouraged research, mainly in Europe and the United States. The researches indicate that the use of pesticides causes diseases to those who handle them, to consumers of products on which pesticides were used, as well as their descendants (GHISELLI and JARDIM, 2007). Since the late 70s, the use of pesticides in Brazil has intensified (FARIA, 2009).

Due to the lack of and difficulty of access to information, scientific evidence concerning the contamination caused by pesticides and their effects are generally ignored. Hence the need for the integration of scientific knowledge and tools to access data in order to elicit knowledge and bring about changes in attitude and lifestyle. This can result in the promotion of health as well as care for the environment. In this context, ontology can be used to represent knowledge about pesticides and about health problems related to the indiscriminate use of pesticides.

The work developed and described here aims to model an ontology, called OntoTox, in order to facilitate the representation of knowledge in the field of poisoning and diseases caused as a consequence of the indiscriminate use of pesticides.

The sections in this paper are presented as follows: in the next section, the methodology used to developed this work is describe; in the Pesticides and Related Diseases section, a definition of pesticides is given together with the consequences that indiscriminate use of pesticides may pose to human health; the Ontologies section briefly describes the methodologies proposed by the available information for the development of ontologies, languages designed to formalize and represent ontologies, and Protégé, a well known tool for its utility; in the Related Work section, some studies are listed, proposing the use of ontologies for the representation of knowledge in a specific field; the Development of the OntoTox section describes the steps followed in the construction of this ontology. Final considerations are presented at the end.

## 2 MATERIALS AND METHODS

Initially, research on the topic ontology, methodologies, tools and languages for the development of ontologies and also about diseases derived from misuse of pesticides were performed. The OntoTox ontology was created following the steps of the methodology Methontology (FERNANDÉZ et al., 1997) and 101 Method (Noy and McGuinness, 2001), based on the requirements collected from two experts in the health field and two of the area of pesticides.

The tool used was Protégé, which is available for free use and was able to assist in the construction of the proposed ontology. The language used for building the OWL ontology was 2.0 in conjunction with RDF and XML as the standard Protégé tool.

The proposed methodology involved the following steps: 1) literature review; 2) analysis of existing ontologies; 3) definition of competency questions that the ontology should answer; 4) creation of ontology; and 5) evaluation of created ontology.

## 2.1 PESTICIDES AND RELATED DISEASES

Pesticides are used in agriculture around the world today but, during World War II, they were used as chemical weapons. Mustard and nerve gas, among others, were used by the Americans and Germans to defoliate tropical forests (BULL and HATHAWAY, 1986). DDT was widely used during this period for the control of lice on soldiers and later as a pesticide in agriculture as well as in public health.

In Brazil, after the Green Revolution in the 60s and 70s, pesticides were introduced to increase agricultural production through the invention and dissemination of new seeds (OCTAVIANO, 2010). In 1975, the Brazilian government launched the National Plan for Agricultural Development, making the purchase and use of pesticides by farmers compulsory, in order to gain access to credit for agriculture. Thus, Brazilian agriculture became dependant on the use of pesticides, which contributed towards the growth of the chemical industry in the country (FERREIRA, 1999).

The adverse consequences of the increasing use of pesticides on human health and the environment have been reported by Bitman and Cecil (1970), Nelson et al. (1978), McLachlan (1980, 1985), Hertz (1985), Richardson and Bowron (1985). The impact on health and the environment results in great social, environmental, economic and political concern. Adverse health effects are usually related to problems with the skin, the eyes, the gastrointestinal tract, the nervous system, the development of tumors and even effects on the endocrine system (CARLSEN et al., 1993).

In Brazil, studies of farmers exposed to pesticides showed high mortality rates due to stomach, esophagus, larynx, and mouth cancer as well as leukemia (MEYER et al., 2003).

Estrogenic or anti-androgenic effects caused by pesticides have also been reported, with the following consequences: infertility, cryptorchidism and hypospadias (ALVES et al., 2007). A study by Trapé (2009) reports that the pesticides which cause most concern to human health are organophosphates, carbamates, pyrethroids and organochlorines, dithiocarbamates fungicides, and phe-noxyacetic herbicides (2,4 D), glyphosate and paraquat.

## 2.2 ONTOLOGIES

According to Clark (1999), ontologies can be considered the materialization of the level of knowledge. They enable automation of the interpretation of the meaning of the information contained in documents (SCHIESSL, 2007) and present themselves as an important tool for using with the Web, because they are reusable and allow for the unification of information in their domain.

The construction of ontologies is based on methodologies, such as Uschold and King (1995), Grüninger and Fox (1995), Noy and McGuinness (2001) and Methontology (FERNANDÉZ et al., 1997).

Languages have been created to formalize and represent ontologies. Among these, the following are worth mentioning: the OIL (Ontology Inference Layer), DAML + OIL, and OWL. SPARQL (W3C, 2013) is a query language for RDF and can be used to express queries across diverse data sources.

The OWL language (W3C, 2009) is derived from OIL and DAML + OIL and consists of a directed evolution of languages for building ontologies. It was developed for representing ontologies and was created in order to describe classes and relations between them, also allowing these classes to be reused or inherited in Web documents and applications. OWL already has three sub-languages, OWL Lite, OWL DL and OWL Full.

According to the next section, the Protégé tool is the most used, and is quite adequate and complete for the purpose, since it allows the combination of several plugins and also uses the OWL language.

## 2.3 RELATED WORKS

Table 1 shows some related works.

Table 1 – Works about ontology of diseases

Ontology	Authors	Objectives	Methodology/ language	Tool
OntopNefro	Bentes Pinto et al. (2009)	It consists of an ontology of images in the field of nephrology	Mehontology / OWL	AKTIVE and Protégé
Ontonegri	Oliveira and Dias (2011)	It is a domain ontology for public health, specifically for neglected diseases	101 Method/ OWL-DL	Protégé
ONTs	Medeiros et al. (2008)	It integrates heterogeneous databases from different information systems used by the Municipal Health Department in Natal, Brazil	Mehontology / OWL	Protégé
DST	Farias et al. (2006)	It manages knowledge in health care related to sexually transmitted diseases (STDs)	Mehontology	Protégé
IDO	Goldfain et al. (2010)	It is a core ontology (the "Core IDO") to encompass terms common to all infectious diseases, ensuring the interoperability of ontology extension (as IDOMAL)		
IDOMAL	Topalis et al. (2010)	It is focused on Malaria, including its clinical and epidemiological aspects	BFO (Basic Formal Ontology) (BFO, 2014)	OBOEdit2 (OBOEdit2, 2014)

Source: elaborated by the authors

The ontologies presented in Table 1 propose the representation of a knowledge base in the health area, focusing on diseases and their causes and symptoms. In this context, the OntoTox contributes with a complementation in the base of symptoms identifying diseases and their causes related to the misuse of pesticides.

### 3 RESULTS AND DISCUSSION

OntoTox was developed using OWL-DL language and the Protégé tool, following the Methontology and the Noy and McGuinness methodology. Considering the steps taken for the development of OntoTox, the 101 Method stands out in the definition of concepts, attributes and relationships, while Methontology discusses the development of the ontology, as a whole.

The modeling of this ontology was done according to the following steps: planning and specification, acquisition of knowledge, conceptualization, formalization, evaluation and documentation.

#### 3.1 PLANNING AND SPECIFICATION

These two steps define the domain of this ontology, its main objectives (representation of knowledge about diseases and poisoning caused by improper use of pesticides), probable users (students and specialists), tasks (activities defined in the Methontology and in the 101 Method) and the necessary resources for its development (Protégé tool, OWL DL language and experts to feed the ontology).

#### 3.2 ACQUISITION OF KNOWLEDGE

For the acquisition of knowledge, it was necessary to access several studies on pesticides and, in particular, on diseases that develop over a period of time, after exposure. The Manual for the Surveillance of Health of Populations Exposed to Pesticides (PAHO) (OPAS/OMS, 1996), issued by the Pan American Health Organization, is well consulted by the toxicology sectors and served as the basis for structuring part of OntoTox.

The SEAB – Paraná state's Secretary of Agriculture and Food Supply (SEAB, 2014) website was used as the basis for collecting information about most pesticides, target groups and cultures considered in the ontology.

In order to facilitate the organization of concepts and the implementation of activities at the conceptualization phase, the "competency questions" (GRÜNINGER; FOX, 1995) that should be answered by the ontology were formulated. These competency questions guided the development of the ontology from the beginning until its final evaluation. In OntoTox, these questions include, in addition to related diseases, the identifying information on agrochemicals or pesticides. The competency questions that OntoTox answers are:

- What pesticides (active ingredients) cause “liver damage”?
- Which groups of pesticides cause “liver damage” in cases of poisoning?
- What are the symptoms of poisoning by “organochlorine insecticide”?
- Which groups of pesticides have “muscarinic effects” in cases of poisoning?
- What are the symptoms of the “muscarinic syndrome”?
- Which groups of pesticides have the symptom of “cholinesterase inhibition” in case of poisoning?
- Which groups of pesticides can cause “estrogenic effects” in cases of poisoning?
- Which groups of pesticides cause “nicotinic effects” in cases of poisoning?
- What are the symptoms of “glyphosate Herbicides (glycine)” poisoning?
- What are the symptoms of “pyrethroids Insecticides” poisoning?
- Which groups of pesticides cause “neurological symptoms” in cases of poisoning?
- What groups of pesticides, in cases of poisoning, correspond to the following symptoms: hypotension, fatigue, hypothermia and hyperpigmentation?
- What pesticides (active ingredient) are risk factors for lung cancer?
- What are the symptoms of poisoning by the insecticide “aldicarb” (Carbamate)?
- What are the symptoms of “pyrethroids insecticide” poisoning?
- Which target groups can be combated with the pesticide “Curinga”?
- What are the synonyms of the target group known as “yellowing”?
- What are the registered target groups and their respective scientific names?
- What is the active ingredient of the pesticide “Captan 200 FS”?
- What is the registrant company of the pesticide “Samurai”?
- Which pesticides are marketed by the company “Milenia”?
- What pesticides contain the active ingredient “cypermethrin”?
- What crops can be treated with the pesticide “Samurai”?
- Which target groups can attack the “corn” crop?
- Which registered pesticides can kill the “apple moth”?
- What are the recommended pesticides to combat the “Southern green stink bug”?
- What are the common names of the target group known by the scientific name “Pythium spp”?



### 3.3 CONCEPTUALIZATION

The concepts required to build this ontology were defined at this stage, the most laborious step in the process of its construction. The main idea of OntoTox is to search for symptoms that identify possible pesticide poisoning. This poisoning can be acute, which is represented by the intoxications class, or chronic, represented by the diseases class. Only the intoxications class is related to the symptoms class, which is divided into six sub-classes of other symptoms related to the systems and apparatus of the human body.

Since this ontology focuses on diseases and poisoning caused by the use of pesticides, 'pesticides' is the main class due to the centralization of information, as can be seen in Figures 1 and 2. This class has relationships with most other classes. The pesticides class has sub-classes: fungicides, insecticides, herbicides and other groups. The 'fungicides' class represents pesticides that act to combat fungus. The 'herbicides' class represents pesticides that are intended to exterminate weeds. The 'insecticides' class represents pesticides that are designed to combat insects, larvae and ants. The 'other groups' class represents pesticides that belong to other groups not covered in the previous three classes.

The 'diseases' class represents diseases that are related to the consequences of misuse of pesticides. These diseases are the formalization of chronic intoxication. In this ontology, the symptoms are not associated with this class since treatment is not the objective, but the relationship of health problems associated with pesticides.

### 3.4 FORMALIZATION

The OntoTox ontology was formalized in the environment of the Protégé tool using OWL DL language. At this stage, the classes of the ontology were instantiated using interfaces created in Protégé. Figure 3 illustrates one of the interfaces of the Protégé tool in the case of the 'pesticides' class.

The instantiation of the ontology covered only enough data so that it could be safely evaluated. Therefore, we selected data involving groups with a higher incidence of pesticide poisoning cases, such as the insecticides groups of 'carbamates', 'organochlorines', 'organophosphates' and 'pyrethroids', and the herbicide group Glyphosate. The data were limited to pesticide products marketed in the State of Paraná (South of Brazil). They were also limited to a small enough group in order to enable a correct return, or not, from the queries.

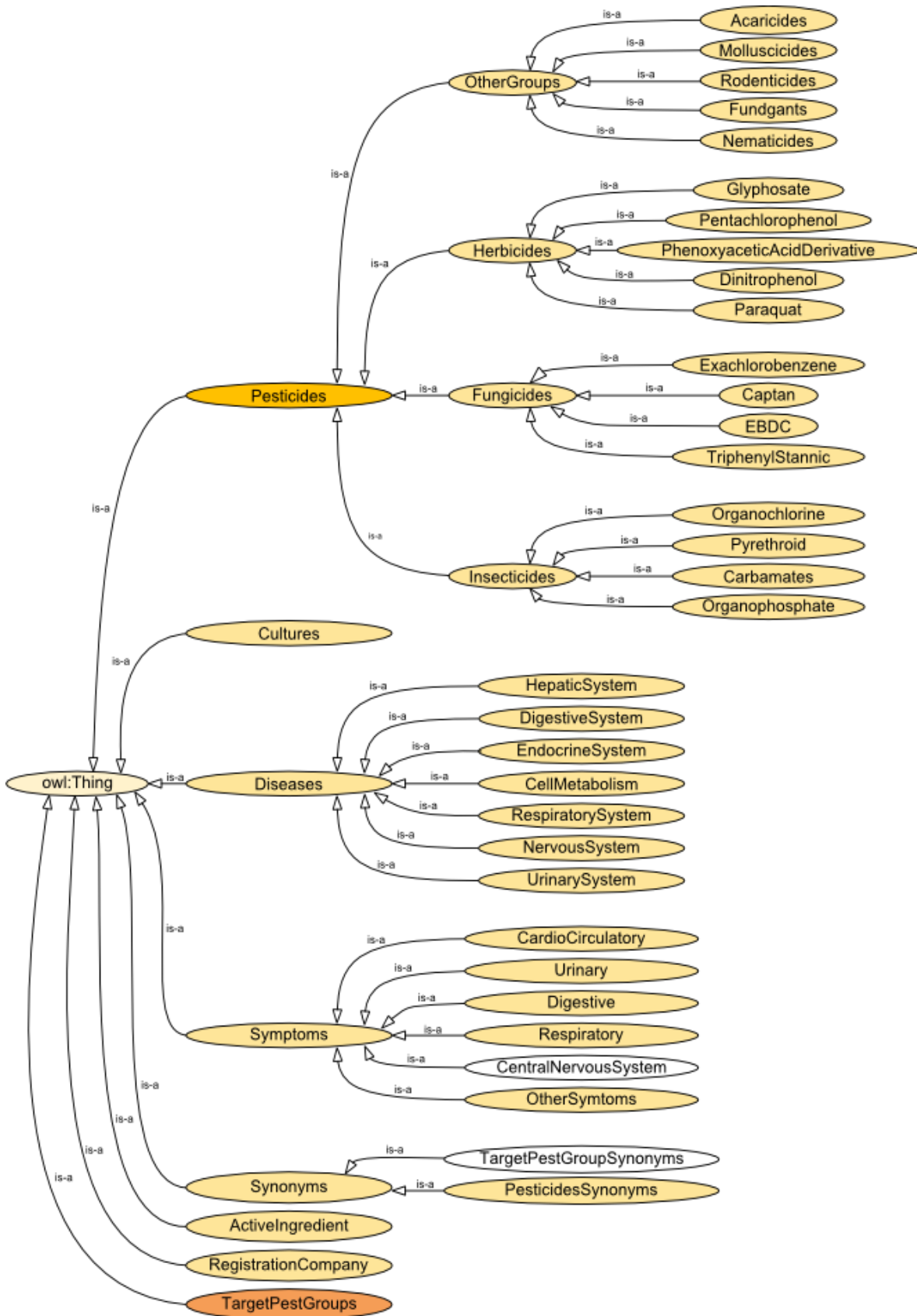


Figure 1. OntoTox class hierarchy  
 Source: elaborated by the authors

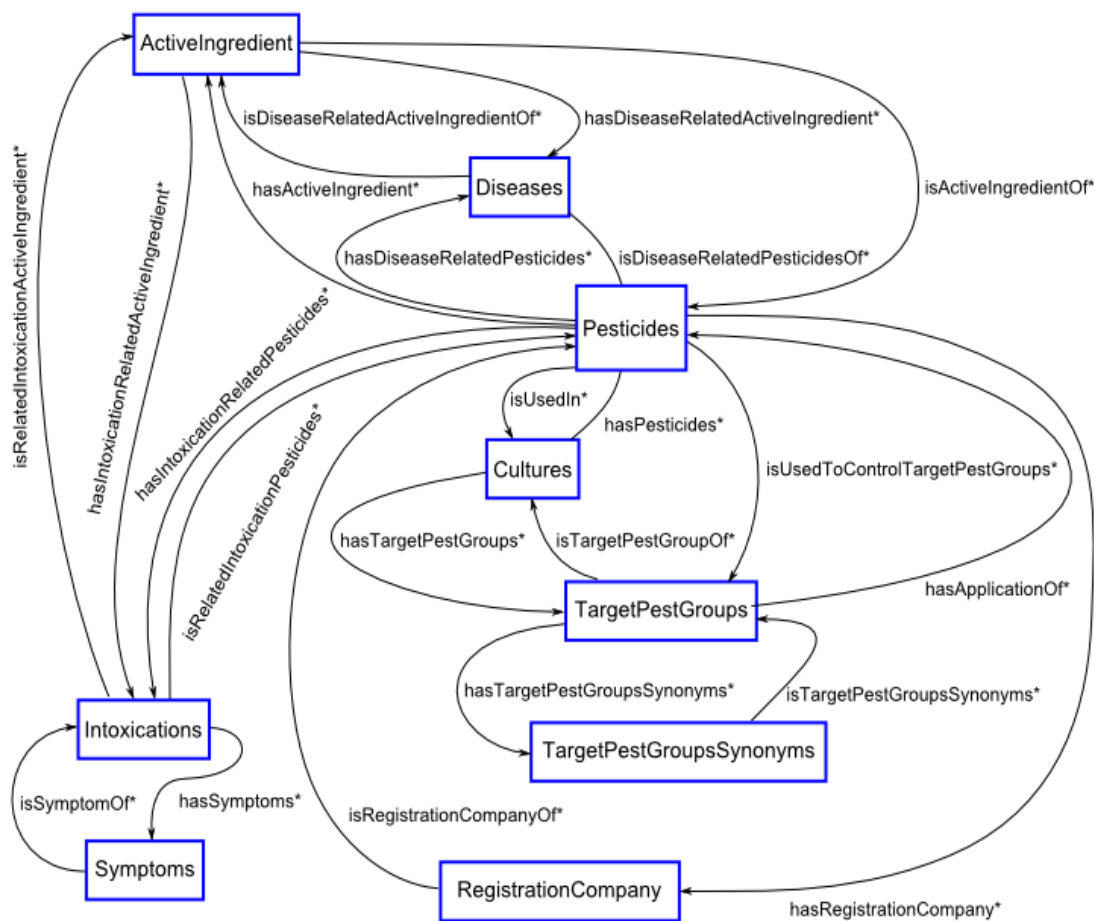


Figure 2. OntoTox classes and their relationships

Source: elaborated by the authors

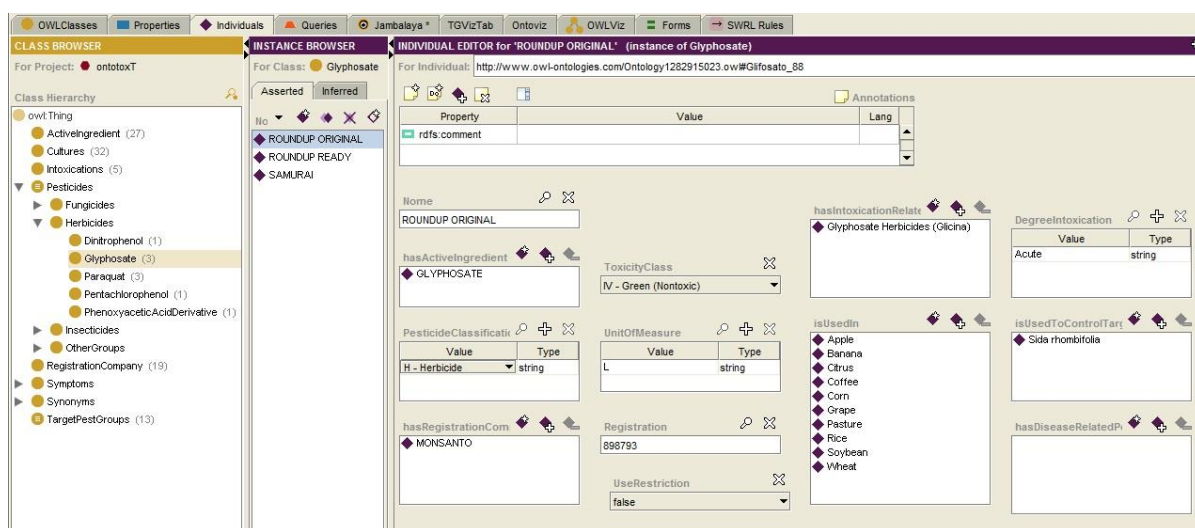


Figure 3. Protégé interface for inclusion of the instance of herbicide glyphosate "ROUNDUP ORIGINAL" of the class pesticides

Source: screen shot of software window

### 3.5 EVALUATION AND DOCUMENTATION

The ontology was evaluated using the data-driven approach (BREWSTER et al., 2004), which suggests the comparison of the ontology with a set of data or documents about the knowledge domain, checking to what extent the domain is represented by the ontology. In this case, classes, sub-classes and properties represented in OntoTox were compared with the information contained in the Manual for the Surveillance of Health of Populations Exposed to Pesticides (OPAS/OMS, 1996) and the pesticides database of the Paraná state's Secretary of Agriculture and Food Supply (SEAB, 2014). This step also included the responses to questionnaires administered to five experts in the fields of health and agronomy. They were structured on competency questions, 15 questions covering health care and 12 in the field of agronomy. The questionnaire was administered to three experts in the field of health and two in the field of agronomy, who suggested some adjustments. After collecting the questionnaires, the following points were considered (measured):

- Are the terms used in the ontology correct?
- Does the hierarchy created reflect reality?
- Are the competency questions in accordance with the purpose of the ontology?
- Is the vocabulary used consistent with the domain?
- Does the ontology answer the “competency questions” correctly?

Among the suggested adjustments is a change in the name of the class ‘TargetPestGroups’ which was originally named ‘pest’. Symptoms of poisoning considered relevant to be addressed, such as, muscarinic and nicotinic syndromes were also included. The ontology was adjusted to these and several other points mentioned after an analysis by the experts on the return of the questionnaires. After the second analysis, the ontology was considered almost complete, except for two questions suggested by one of the experts in the field of agronomy.

The Protégé Query tab was used in order to formulate and implement the competency questions. Figure 4 illustrates one of the competency questions of the questionnaire, using the Query tab of Protégé (Which groups of pesticides cause “liver damage” in cases of poisoning?).

All classes of the ontology were involved in the evaluation. Both the formulation of questions and the responses were evaluated. The ontology answered all the evaluated questions appropriately as expected.

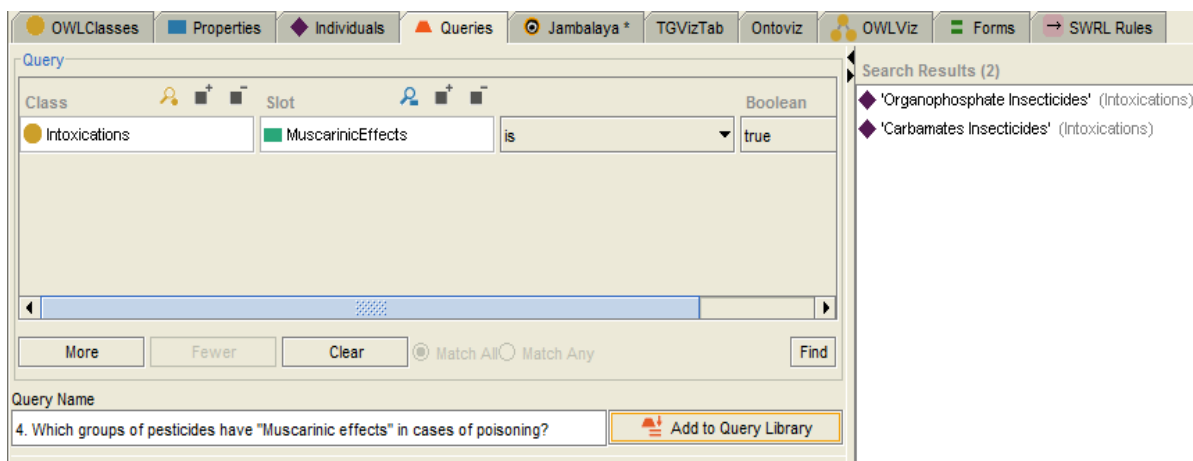


Figure 4. Example of a competency question for the evaluation of OntoTox  
Source: screen shot of software window

## 4 CONCLUSION

This paper presented a report about the construction of an ontology of diseases caused by improper use of pesticides. The development of this ontology was motivated by concern with the increasing degradation of the environment due to the use of pesticides and their effects. Thus, the main contribution of this paper is the OntoTox ontology, which represents knowledge about pesticides as well as the diseases and poisoning caused by their improper and indiscriminate use.

The OntoTox ontology was developed with the guidance of five experts in health and agriculture. It was based on the Manual for the Surveillance of Health of Populations Exposed to Pesticides, issued by the Pan American Health Organization (PAHO), and SEAB's website.

The evaluation of the OntoTox ontology was performed using the data-driven method, which consists of a comparison of documentation on the area addressed. Questionnaires were administered to assess the responses to the defined competency questions. During the evaluation phase, the ontology was adjusted to accommodate the suggestions made by experts in the areas of health and agriculture. It was also necessary to adjust the competency questions and the questionnaires. After these adjustments, OntoTox was considered by the experts as a valid representation of knowledge about pesticide poisonings and diseases caused by their use.

The structure of OntoTox allows access by systems that handle information on pesticide poisoning, because it was based on work done in an intoxication control center. It can also be used by systems that require information about the registration of pesticides.

In future, OntoTox can be extended to include more information resulting from research on the subject. This ontology can also be reused in the creation of other ontologies on the themes, "poisoning" or "pesticides".

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