
PROTOCOL DATA MANAGEMENT IN BIOLOGY LABORATORIES: proposal for the development of an information management system

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Abstract

The main objective of information organization is to disseminate information objects effectively to users. It is a complex but important task that uses elements such as the form and informational content of documents, and it is a prerequisite for an efficient organization. Research laboratories are examples of organizations that have a diverse and complex set of data that must be well organized. Their flow of information needs to be mapped to properly identify people, information sources, technology used as well as products and services. In this work we describe the development of the FluxP system to organize information on protocols from a Biology Research Laboratory — The Animal Venoms and Toxins Laboratory (LVTA) from the Federal University of Minas Gerais – Brazil. FluxP is able to manage protocol data and makes it simple to store and retrieve protocols to aid in the experimental work, increasing the reliability of experiments and helping reduce experimental errors. By establishing a central repository for protocols FluxP prevents protocols from being misplaced or lost and by categorizing them FluxP makes it simple to retrieve protocols based on keywords. The system is currently being used by LVTA to manage a collection of 50 protocols, and can be easily adapted for other laboratories.

Keywords: Information management; LIMS; Biology Laboratory; Research Protocols.

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1 Introduction

1.1 Knowledge Organization Systems (KOS)

The effectiveness of information retrieval is strongly related to information organization systems. Knowledge Organization Systems, KOS, systems to perform this task, are instruments used to index and browse collections. A KOS is a set of elements, usually structured and controlled, that can be used to describe (index) objects, browse collections, etc. Typical examples of KOS are thesauri, classifications, subject heading lists, and taxonomies (Skos 2004). KOSs make domain knowledge explicit and enable information organization and retrieval (Vickery 2008). They make it possible “to delimit the use of terms and define concepts and relationships of some knowledge area, in a shared and consensual way.” Bräscher and Carlan (2010 p. 149).

Dahlberg (1993 p. 211) defines knowledge organization as "the science that systematically structures and organizes knowledge units (concepts) according to their inherent knowledge elements (characteristics) and the application of these concepts and classes of concepts ordered to objects/subjects."

Concepts or notions are units of knowledge, as recalled by Dalhberg (1993), they are fundamental elements of knowledge organization systems that, based on the characteristics of existing objects in a given domain, are grouped and ordered into classes.

Knowledge Organization Systems are products of knowledge organization that, according to Bräscher and Carlan (2010 p. 149) consist of a “modeling process that aims to build knowledge representations”. Furthermore the authors also point out that knowledge organization systems comprise “types of conceptual systems, or types of knowledge representations, fruits of the knowledge organization process.” Bräscher and Carlan (2010 p. 149). In this sense, as conceptual systems, these systems are used to represent the thematic point of view or to represent the content of informational objects. These tools are used in document classification and indexing processes and set standards for the conversion of concepts into terms that represent document subjects. Another important aspect of these instruments is the communication function of knowledge organization systems, which enable users to interact with systems, as pointed out by Boccato, and Fujita (2006). The authors state

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that it is an “instrument of communication between information, the information system and the user, it must ensure access to this information, enabling its proper retrieval” Boccato, and Fujita (2006 p. 18).

Classification and indexing processes are related to information organization. According to Jacob (2004 p. 522) “classification as process involves the orderly and systematic assignment of each entity to one and only one class within a system of mutually exclusive and no overlapping classes.” Establishing each subject in a specific class is part of both indexing and classification activity.

1.1.1 Categorization

According to Jacob (2004 p. 518) Categorization is the process of dividing the world into groups of entities whose members are in some way similar to each other. Categorizing consists of classifying objects by grouping them into classes by similarities and differences. Similarities and differences according to Lima (2010) lead to the creation of new knowledge and “the brain shapes structures that mirror the external environment in a categorical form.” Lima (2010 p. 110). In this sense, the interaction with the environment allows us to categorize objects in a contextualized way from the experiences of a world model and culture, as well as to reflect on these categories and make statements about the objects from the characteristics that were determined to group them.

In Information Science the categorization exercise is performed both in the knowledge organization activity and in the information organization. In the first case categorization occurs in the conceptual modeling of a domain whose model has a vocabulary formed by terms and their relationships. These terms correspond to the verbal form of the concepts, carry the proper meaning of the domain, are directly related to the specific context of this domain and are allocated in a class or part of a category.

1.2 Information Organization

In all institutions the organization of information contributes to giving access to information objects. Access to informational objects is a major concern of Information Science. Access is made possible by searching and retrieving information in information systems.

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It is important to highlight the role of the organization, the content, the representation of the information and the instruments that allow the implementation of the operations for the representation of the elements for the cataloging. This set of instruments includes cataloging codes for the representation of descriptive elements of objects, classification systems and indexing languages that are essential for the representation of information from the thematic point of view. All of these tools are used for organizing information and contribute to giving visibility to the content and the metadata of the descriptive, structural, administrative and preservation types that are required to manage and retrieve information.

The organization of information is the arrangement of traditional or electronic collections, accomplished through the physical and content description of their informational objects (Café, and Sales 2010). According to these authors there are two different dimensions to the process of information organization: descriptive and thematic. The first dimension, descriptive, deals with the elements of the form of the documents, making it possible to identify the attributes of the informational objects. The descriptive dimension creates a representation of documents which describe their content in addition to their extrinsic characteristics. The second dimension, thematic, corresponds to the informational contents, focusing in the analysis, identification and representation of the subject matter of these objects. Both dimensions have been investigated in this paper. This process deals with the “organization of objects in collections as they appear in libraries, museums and archives as the production of instruments to retrieve information derived from these objects through physical and content description” (Bräscher, and Carlan 2010; Café 2008 p.7).

The main objective of the information organization is to disseminate the information objects to the users. To achieve this goal there are processes, methodologies, standards and instruments that allow the description, representation and integration of data of these objects to retrieve information in all its possible attributes, as well as the aspects that involve its content. In addition to retrieving documents, other interests can be perceived by the community that has an interest in certain objects. These interests also require the access to fragments of information of certain documents, the identification of the meaning of certain data, the identification of the relationship between objects or even the use of a common vocabulary between users and information retrieval systems.

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The variety of information resources generated, the difficulty of access, the need to improve information dissemination and problems in information retrieval are variables that contributed to the creation of new shapes for the structured representation of information. In this context the metadata emerged to assist in the standardized description.

1.3 Metadata

Metadata are resources that enable the representation of information of the various aspects present in information objects. (Borbinha 2003) presents the broad scope of metadata representation. For the author the contents of objects can be described. Some examples would be keyword indexing, classifying information structure according to layout, format or size, recording data about the author, stating creation date, protection, and others. In addition, it is possible to disclose information about the conditions of use, identifying for example authorization required for access, price, among other elements. Besides describing and representing objects, metadata is fundamental for information retrieval.

According to the Dublin Core Metadata Initiative (DCMI) definition. Metadata is “Data associated with an information system or information object for the purposes of description, administration, legal requirements, technical functionality, use and preservation”. This definition clarifies the role of metadata in making reference to description processes, a typical activity of information organization for Information Science. In addition, it expands metadata roles by pointing to legal requirements and functionality, and innovates by mentioning digital preservation.

Faced with so many roles, we highlight the diversity of objects that have or demand a metadata standard to describe them. These objects can be of traditional types such as thesis, dissertations, geological maps, images, sounds or those present in biological research laboratories. This study will use metadata to describe the research protocols used by researchers.

1.4 Information Organization for Research Laboratories

Research laboratories have a diverse and complex set of data that must be well organized for them to function properly. This is a very heterogeneous group and in this scenario

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each laboratory has a specific flow of information that is peculiar to it. This flow needs to be mapped identifying people, information sources, technology used as well as products and services, with the objective to compose a structured set of activities related to how information and knowledge are obtained, distributed and used (Silva, and Tomaél, 2007).

Several tools have been used to collect and manage all the information associated with research laboratories. The use of computational tools to aid in this task have been described, including the use of Electronic Laboratory Notebooks (ELNs) and Laboratory Information Management Systems (LIMS) (Melo, *et al.* 2010).

An ELN is a system to create, store, retrieve and share fully electronic records from laboratory experiments in ways that meet all legal, regulatory, technical and scientific requirements (Rubacha; Rattan and Hosselet 2011). It is usually used to substitute conventional paper-based notebooks. ELNs have many advantages when compared to their paper counterparts. Information can be easily modeled, displayed, transmitted, searched and indexed. The same advantages can be described for LIMS, complex computer systems used to store and manage laboratory data. However, their main focus is guaranteeing the quality of the processes and assure that results are produced consistently and reliably. Additionally, they control the entire data life cycle, from acquisition and storage to analysis and reporting (Hinton 1995; Melo *et al.* 2010; Avery, McGee, and Falk 2000).

Although ELNs and LIMS can both be used to handle lab information effectively, complementing each other's functionality if wanted, LIMS and ELNs are best suited for structured and unstructured data respectively. Nonetheless, as these systems are constantly evolving, many functionalities from ELNs are being included into LIMS and vice versa making it harder to define a proper distinction. LIMS can be used as ELNs if they support registering and sending information retrieved from different data sources. For LIMS and ELNs is important to support the internal lab process in an efficient manner and ensure data integrity (Machina, and Wild 2013; Sydor, and Kim 2017).

To develop either LIMS or ELNs to work as biological data processing, medical expert systems, e-science and other lab related applications it is necessary to implement well-thought conceptual structures to store and retrieve all data involved in the research. These structures

can be developed using informational tools through interactions with users and with the aid of computer systems. This development can be made from scratch or by refining previous structures. In this work we describe the development of a system to organize information on protocols from a Biology Research Laboratory – The Animal Venoms and Toxins Laboratory (LVTA) from Federal University of Minas Gerais – Brazil. This system uses SIGLa, a workflow based LIMS as basis.

2 Methodology

To perform the empirical part of this study, the following methodological procedures were implemented: technical visits, construction of a tool to manage the protocols (FluxP forms), categorization of the protocols used in the LVTA and experimental tests with 3 researchers from the LVTA as described below.

In order to analyse the informational structure of LVTA a diagnosis was carried out through technical visits and discussions with lab members about the main needs of the lab regarding information storage and retrieval.

The technical visits were carried out with the objective of identifying the informational resources present at the LVTA. Each of these objects contains a significant amount of information and is directly related to the activities performed in the biological laboratory. These information resources include: a) inputs, reagents and equipment used; b) available bibliographic resources; c) team involved in the laboratory; d) available biological protocols; e) workflow developed in the laboratory. Identifying and storing the representations of these informational objects helps in creating an information retrieval system and enables information to be used to generate new knowledge. It is noteworthy that the focus of this study was on item d), the biological protocols used in research.

One aspect of the informational needs of this laboratory to be addressed is the management of research protocols used by researchers. These protocols are stored today throughout the laboratory on students and researchers paper notebooks and computer files without any kind of structured system that would allow retrieval or searches. Therefore, an

important step on the informational organization for LVTA is the construction of a tool to manage such protocols.

2.1 Protocols

In Natural Sciences a protocol is a predefined procedural method designed to support the conduct of experiments. Protocols standardize a laboratory method to ensure successful replication of results by others in the same laboratory or by other laboratories. Its content has a complete description of procedures, equipment, instruments, chemicals and other supplies used besides study objectives, reasoning for experimental design, reasoning for chosen sample sizes, safety precautions, and how results were calculated and reported. LVTA uses currently 50 different protocols that were used to design and test the proposed tool. In order to organize protocol data, an analysis of documents of this type was carried out. Descriptive fields of these documents have been identified, which were used as metadata for the creation of the electronic forms for insertion and storage of this information in the protocols management system (FluxP). The metadata identified are as follows:

Table 1- Metadata characterization

Metadata type	Metadata	Metadata description	Database Type
Administrative	Creation date*	Original date of protocol insertion	DATE
Administrative	Modification date*	(Optional) Protocol last Modification date	DATE
Administrative	Created by*	User that registered The protocol	STRING
Administrative	Changelog*	Protocol modification History	TEXT
Descriptive	Title	Protocol title	STRING
Descriptive	Author	Protocol authorship	STRING
Descriptive	Category	Protocol classification	STRING
Descriptive	Description	Protocol description	TEXT
Descriptive	Reagents	List of Reagents	TEXT
Descriptive	Equipment	List of Equipment	TEXT
Descriptive	Procedure	Procedure for executing the protocol	TEXT
Descriptive	Expected Results	Expected results for executing the protocol	TEXT

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Descriptive	Observation	Observations	TEXT
Descriptive	References	Bibliography References	TEXT

Source: research data

Metadata assigned with * are automatically generated by the system and control the versioning of the protocol for organization administration and information management.

2.1.1 Form for Protocol organization in FluxP

The LIMS SIGLa was used as the framework to construct the forms for the protocol organization tool – FluxP. SIGLa is a workflow based LIMS, that incorporates a workflow management system, making it possible to create and manage customized workflows (Melo, et al 2010). A XML Process Definition Language (XPDL) file was constructed using a Workflow Editor and uploaded in SIGLa, which creates the forms that are filled by the users with protocol information.

2.1.2 Protocol Categories

Protocol forms have a Category field that helps organize groups of protocols. In 2016 a study of knowledge organization and management was carried out to develop a categorization system for the protocols used in the LVTA, in order to classify them by subject and provide information retrieval. Searches were conducted using the following terms in portuguese “protocolos biológicos”, “sistemas de classificação para ciências biológicas” and “gestão da informação e conhecimento para ciências biológicas” in the “Portal de Periódicos da CAPES (Coordenação de Aperfeiçoamento de Pessoas de Nível Superior)”, in the eletronic database SciELO (Scientific Eletronic Library Online), and also in the thematic groups 2 and 3 (“Organização e Representação do Conhecimento” and “Gestão da Informação e Conhecimento”, respectively) of “Encontro Nacional da Associação Nacional de Pesquisa e Pós-Graduação em Ciência da Informação (ENANCIB)”. The search string “protocolos biológicos” in the “Portal de Periódicos da CAPES” resulted in the discovery of a specific database for indexing of this nature called *Wiley’s Current Protocols*. This journal is a publication that lists biological experiment protocols, published by John Wiley Sons.

Through the analysis of the categories available in the journal *Wiley's Current Protocols*, a classification structure with 26 categories and 376 subcategories was organized. An experimental classification of a sample with 10 protocols randomly chosen from the available LVTA protocols was conducted. After performing this experimental classification, it was found that the categories available in *Wiley's Current Protocols* were adequate for the classification of laboratory protocols. From this realization that *Wiley's Current Protocols* categories could be used to classify LVTA protocols, a unique code identification structure based on Current Protocols was developed. (Appendix, Figure 1).

The subset of categories from *Wiley's Current Protocols* was chosen discussing with LVTA's researchers that helped to select the ones that relate to protocols used by the laboratory. After the categories were chosen a simple word matching between protocol name and/or description and categories was performed using 50 protocols. In case of no match a category was manually associated to a protocol. In case of match the category association was validated by a researcher. Associations considered invalid required manual association for correction. After this procedure the categories became available in the forms to be used to classify other protocols as these would be inserted in the system. (Appendix, Figure 2).

3 Results

3.1 Protocols

The protocols are presented to the user as a list in which the instances of protocols registered in the system are represented by the lines of the table and the columns represent the attributes that describe the protocol (Appendix, Figure 3). For the initial tests 20 protocols have been loaded in the system. The protocols can be visualized by the users clicking on Protocols in the main page, then clicking on the magnifying glass icon beside the protocol's name. The visualized protocol can be exported as a pdf file by clicking on the Export button. Additionally, a selection of protocols by category can be made by using a keyword in the Filter all fields box (Appendix, Figure 3)

As the electronic protocol form can have as many attributes as required and the content of each one can be large enough to have all the information needed to describe the protocol

properly, all the data may not be fully shown at first (Appendix, Figure 2). However, this kind of visualization helps the user to have a glimpse of what is registered in the system. In order to access the full content of each protocol the user may click on the magnifying glass icon (Appendix, Figure 4).

3.2 Protocols Categorization

Descriptors on the protocols have been used to help choose the category to which each protocol belongs. The Category field was used to classify the protocols while other descriptive fields have been used to index the textual content of the protocols to allow information retrieval using FluxP. All fields were validated by the users using questionnaire application and interviews, in order to produce a real representation of the protocols that are created in the laboratory. Like Dublin Core or other descriptive metadata tool, the definition of this standardization allows flexibility and reflects the reality of LVTA protocols.

In this work we propose a new system to categorize different types of laboratory protocols since no specific tool was found for indexing this type of content and classification systems such as CDU and CDD are very generalist. The aforementioned system is organized in 17 main categories with its subgroups adding to 94 categories that can be used to classify the protocols. Other categories can be added to FluxP as needed.

4 Discussion and Conclusion

The organization of laboratory data is a complex and very important task. Biological laboratories perform complex experiments whose results depend on several parameters, and keeping track of these data can be challenging. Frequently protocols can be misplaced or lost, due to the lack of organization in the laboratory, or to the fact that several researchers, technicians and students use these protocols, and communication between them can be faulty. The loss of a protocol may prevent an experiment from being executed, but the use of an incorrect or outdated protocol can cause experiments to be executed wrong, wasting time and resources in the laboratory.

In this paper we propose FluxP, a system to organize protocol information from biological laboratories that is able to manage protocol data making it simple to store and

retrieve protocols to aid in the experimental work, increasing the reliability of experiments and helping reduce experimental errors. By establishing a central repository for protocols FluxP prevents protocols from being misplaced or lost. By categorizing protocols and making it simple to retrieve them based on keywords FluxP makes it straightforward to identify not only the correct protocol to be used, but also to see in a glance if other related protocols exist. In this way the person executing the experiment will have a higher degree of confidence of choosing the correct protocol. This is particularly useful in research laboratories, since often the technician performing the experiment is a student with little experience and ensuring that the correct information is used is very important. Another advantage of FluxP is that it allows laboratories to share protocols increasing the dissemination of information in a controlled manner. Shared protocols will be tagged with keywords, authorship and other information that will ensure its applicability.

We have implemented FluxP in a Biology Research Laboratory, The Animal Venoms and Toxins Laboratory (LVTA) from Federal University of Minas Gerais – Brazil. The system is currently being used by LVTA to manage a collection of 50 protocols.

Experimental tests were performed with 3 LVTA researchers in order to confirm the how the indexation performed. The researchers who participated in this experiment had to perform 3 searches on the FluxP protocol system using the keywords "protein", "dichroism" and "chromatography" in the Category search field. For all searches, the retrieved protocols were correctly indexed, demonstrating the high accuracy of information retrieval in FluxP. Another discussion presented to the researchers who participated in this experiment was the ease of accessing the protocols through a unified system that allow indexing and later retrieval of information from these documents.

FluxP is flexible enough to be adapted to other laboratories, and future work includes adapting it different types of laboratories and more complex protocols.

5 Availability

The FluxP system can be accessed at www.fluxp.luar.dcc.ufmg.br using the user guest and password gu3st.

Notes

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Appendix

Figure 1 - Sample of FluxP categories and subcategories based on Current Protocols.

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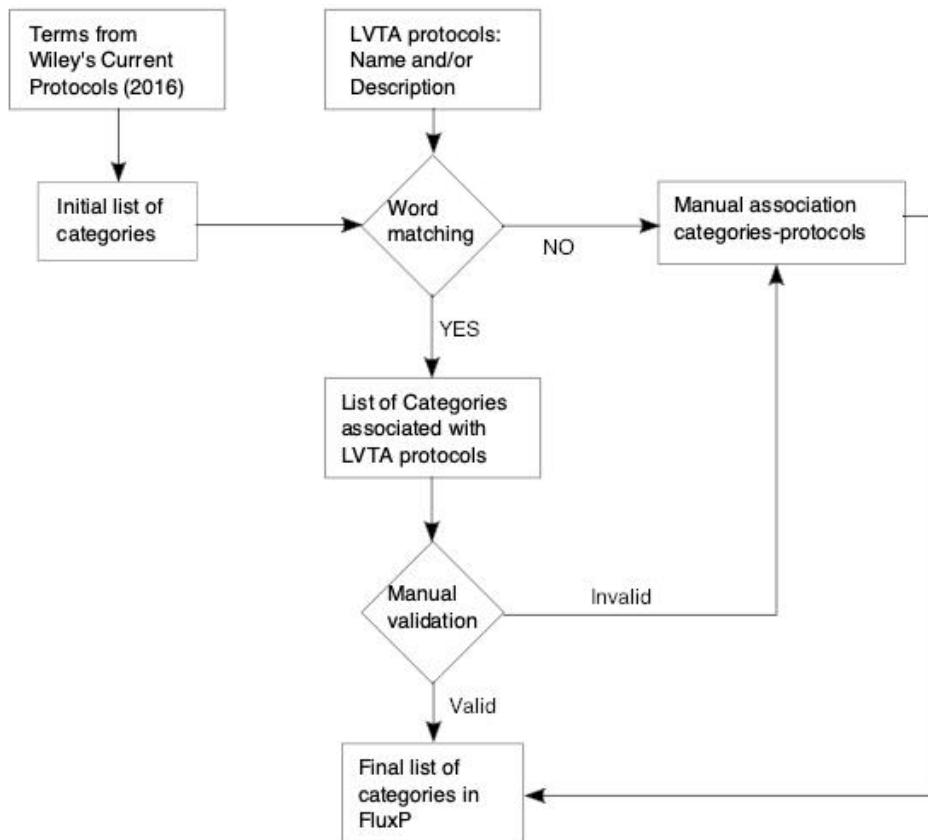
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  <subcategories sc_id="001.001" name="Bioinformatics Fundamentals"> </subcategories>
  <subcategories sc_id="001.002" name="Biological Databases"> </subcategories>
  <subcategories sc_id="001.003" name="Cheminformatics"> </subcategories>
  <subcategories sc_id="001.004" name="DNA Analysis"> </subcategories>
  <subcategories sc_id="001.005" name="Expression Patterns"> </subcategories>
  <subcategories sc_id="001.006" name="Finding Genes"> </subcategories>
  <subcategories sc_id="001.007" name="Finding Similarities and Inferring Homologies"> </subcategories>
  <subcategories sc_id="001.008" name="Genome Variation"> </subcategories>
  <subcategories sc_id="001.009" name="Modeling Structures from Sequence"> </subcategories>
  <subcategories sc_id="001.010" name="Molecular Modeling"> </subcategories>
  <subcategories sc_id="001.011" name="Phylogenetic Trees"> </subcategories>
  <subcategories sc_id="001.012" name="Protein Analysis"> </subcategories>
  <subcategories sc_id="001.013" name="Proteomics"> </subcategories>
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  <subcategories sc_id="001.015" name="Recognizing Functional Domains"> </subcategories>
</categories>
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▼<categories id="003" name="Cell Culture">
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  <subcategories sc_id="003.002" name="Cancer"> </subcategories>
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  <subcategories sc_id="003.006" name="Plants"> </subcategories>
  <subcategories sc_id="003.007" name="Sample Preparation"> </subcategories>
  <subcategories sc_id="003.008" name="Viruses"> </subcategories>
  <subcategories sc_id="003.009" name="Yeasts and Fungi"> </subcategories>
</categories>
▼<categories id="004" name="Chemical Biology">
  <subcategories sc_id="006.001" name="Carbohydrate Modifications, Engineering and Applications"> </subcategories>
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```

Source: research data

Faria-Campos, Alessandra; Dias, Célia; Teixeira, Gabriel; Alphonsos, Alexandre; Leite, Germano; de Lima, Maria Elena; and Campos, Sérgio. “Information organization and representation in biology laboratories: Protocol management in a research laboratory”. *Brazilian Journal of Information Studies: Research Trends*. vol.10, n. 1, 2020, pp.173-189.

Figure 2 - Procedure for selection of Categories to be used in FluxP forms



Source: research data

Figure 3 - List of protocols in the FluxP system filtered using the keyword “Protein”

View	Edit	Delete	Title	Author	Category	Description
			Circular Dichroism	LVTA	Protein Production, Purification, and Analysis	Determination of the secondary structure and folding properties of proteins.
			Protein Concentration Quantitation – The Mini-Lowry Method	LVTA	Protein Production, Purification, and Analysis	Total crude venom, semi-purified fractions and isolated toxin proteins were estimated by
			Peptide Synthesis	LVTA	Protein Production, Purification, and Analysis –	Synthesis of peptides on solid resins by the incorporation of amino acids protected by F
			Western Blot	LVTA	Molecular Biology	Evaluation of protein expression
			Reversed-Phase Chromatography	LVTA	Protein Production, Purification, and Analysis	Purification of synthetic peptides for the removal of possible impurities
			Mass Spectrometry - MALDI TOF	LVTA	Protein Production, Purification, and Analysis –	Technique that measures the mass-to-charge ratio of ions. The results are typically pre
			Ion Exchange Chromatography	LVTA	Protein Production, Purification, and Analysis	In ion exchange chromatography, the stationary phase is highly charged, and charged s
			DIGE	LVTA	Protein Production, Purification, and Analysis –	Difference gel electrophoresis is a form of gel electrophoresis where up to three differen

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15 protocol(s).

Source: research data

Figure 4 - Full content visualization of a protocol in the FluxP system

View Protocol ✕

[Export](#)

Title:
Circular Dichroism

Author:
LVTA

Category:
[Protein Production, Purification, and Analysis](#)

Description:
Determination of the secondary structure and folding properties of proteins.

Reagents:
Trifluoroethanol (TFE)
Sodium dodecyl sulfate (SDS)
N-dodecylphosphocoline (DPC)
Peptide to be tested
Milli-Q water
Nitrogen gas (N2) -- High purity

Equipments:
Micropipettes 1000, 200 and 20 uL
Spectropolarimeter
400 uL quartz cuvettes
Bucket adapter
1.5 ml Eppendorf tubes
1000, 200 and 20 uL tips

Procedure:

1. Prepare titers of peptide compound at 100 ug/ml -- Increasing concentrations of 0% up to 60% TFE.
2. Prepare titers of peptide compound at 100 ug/ml -- Increasing concentrations of 20 uM up to 20 mM SDS.
3. Prepare titers of peptide compound at 100 ug/ml -- Increasing concentrations of 20 uM up to 20 mM DPC.

OBS: For all titers do not forget to prepare the respective blanks where no test compound is added.

4. Add each sample by first reading the blank, the the test compound with the same blank concentration in the spectropolarimeter. Do not forget to use N2 flow during the reading. Readings are in the 260 to 190 range at a scanning of 50 nm/min and an acquisition of 0.2 nm at a time.
5. Wash the cells with Milli-Q water between readings.
Perform data deconvolution using the CRData program.

Observation:
None.

Source: research data