Procedurally Rhetorical Verb-Centric Frame Semantics as a Knowledge Representation for Automated Argumentation Analysis

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Chapter 1

Introduction

1.1 Background

Scientists must routinely review the scholarly literature in their fields to keep abreast of current advances and to retrieve information relevant to their research. However, the volume of online scientific literature is immense, and rapidly increasing. In the biomedical field, the National Centre for Biotechnology Information (NCBI) developed a literature search engine, PubMed[1], to access various databases such as MEDLINE (journal citations and abstracts for biomedical literature), full-text life science e-journals, and online books. In 2010 PubMed repositories consisted of more than 20 million citations for biomedical literature [34]. By 2015 the number of citations had increased to more than 25 million[2]. As a consequence, it has become extremely challenging for biomedical scientists to keep current with information in their fields. This challenge has attracted Natural Language

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[1] http://www.ncbi.nlm.nih.gov/pubmed

[2] http://www.ncbi.nlm.nih.gov/books/NBK3827/

Processing (NLP) researchers to develop resources and automated tools for performing various tasks in Information Extraction (IE) and Text Mining (TM) using online corpora of biomedical articles, and thus enable biomedical researchers to better manage and exploit this volume of data [26]. These research activities have led to the development of a new field, Biomedical Natural Language Processing (BioNLP), a collaboration between the biomedical and computational linguistics/artificial intelligence communities [25].

The types of tasks currently handled by BioNLP systems have generally been aimed at extracting very specific and limited information, for example, protein and gene names and relations [12], and so have been able to rely on relatively simple forms of information extraction. BioNLP has adapted various standard information extraction techniques, including both rule-based (e.g., shallow parsing, syntactic pattern-matching) and Machine Learning (e.g., Support Vector Machines, k-nearest neighbour classification method), to address several text-mining tasks, including extracting: protein-protein interactions (PPI) [31], drug-drug interactions (DDI) [46], gene relationships [27], and protein-residue associations [42].

Although these approaches fulfil some information needs, information extraction systems based on these can only recognize and extract minimal and specific information from biomedical texts. But other, more in-depth and comprehensive, information contained in biomedical texts would be highly valuable to scientists because this type of information can enable validating scientific claims, tracing current research directions in their field, reproducing scientific procedures and so forth. Recently, a new and more challenging information extraction task has been introduced as a means of obtaining these types of detailed information: identifying the argumentation structure in biomedical articles (e.g., [23] and [24]). *Argumentation mining* can be used to validate scientific claims and experimental methodology, and to plot deeper chains of scientific reasoning. Unlike earlier simpler forms of information extraction, here the goal is to identify the structure of argumentative components within an entire text—for example, premises, evidence, conclusions—as well as the relationships between components.

1.2 The Problem Statement

Over the past decade, the focus on argumentation mining has been growing significantly in different areas of Artificial Intelligence (AI) research. The incentive to build Natural Language Processing (NLP) systems to automatically identify and analyze argumentative components in various genres of texts has increased because knowledge of argumentative structure facilitates various tasks such as text summarization ([50] and opinion mining for commercial purposes [63]. The study of automated argumentation analysis has attracted the interest of several communities, including both scientific and computational linguistic researchers. Researchers from Argumentation Theory and Artificial Intelligence have come together to develop this new field of Computational Argumentation in interdisciplinary conferences and publications (e.g., Computational Models of Argument Workshop (COMMA), *Argument & Computation* journal). Various computational studies have been done to analyze different argumentation aspects, including: the structure of valid arguments in legal documents [37], scientific articles ([22], [23] and [24]), and the role of argumentation in multi-agent systems [39]. In particular, researchers are developing automated argumentation analysis systems to enable scientists in the experimental sciences to review and evaluate scientific findings more efficiently, and to help identify whether scientific claims are valid or not, based on their argumentative structure (e.g., [32] and [51]).

In addition to the biomedical field, researchers have worked on argumentation mining tasks in a variety of other domains, mainly: on-line debates [8], legal documents [37], newspaper articles and court cases [16], and product reviews [63]. However, these approaches have lacked consistency in their definitions of argumentation "schemes" (i.e., labels used to identify the different components of an argumentative structure). Moreover, there has been no formal, computationally feasible, semantics for these schemes. As a consequence, it has been difficult to build automated systems that can identify the components of an argument with a high degree of accuracy. And, because of the many different argumentation schemes, it has been impossible to come up with standardized metrics and evaluations of these different approaches.

In this research we will work on the biochemistry domain to develop a formal knowledge representation, *procedurally rhetorical frame semantics*, that can be used for in-depth argumentation analysis, is computationally feasible to implement, and will enable argumentation mining of more-detailed scientific knowledge than is currently available. This will be an important step towards providing researchers in Computational Argumentation working in domains with similar discourse structure with a means of using and evaluating the metrics we will develop. To the best of our knowledge, no research has proposed or incorporated the idea of a semantic frame based on verb analysis to assist in the analysis of argumentation in biochemistry articles.

The structure of the document will be as follows: First, an overview of some theoretical and computational approaches to argumentation are presented in Chapter 2. Then, our proposed approach to argumentation analysis is described in Chapter 3. Next, a description of our methodology is given in Chapter 4 . Finally, a conclusion of this report is given in Chapter 5.

Chapter 2

Related Work

2.1 Argumentation Theory

In this section, we present a brief overview of argumentation and discuss some of the early works on argumentation analysis.

2.1.1 What is Argumentation

Argumentation can be defined as “a verbal, social, and rational activity aimed at convincing a reasonable critic of the acceptability of a standpoint by putting forward a constellation of propositions justifying or refuting the proposition expressed in the standpoint” [59]. The essence of argumentation can be considered as influencing others to gain their adherence to a particular idea [41]. Tindale [52] defined argumentation as “the site of an activity, where reasons are given and appraised, where beliefs are recognized and justified, and where personal development is encouraged”. Arguments have an explicit logical structure, for example, claims that are backed with reasons, which in turn are supported by evidence, leading to conclusions [53].

Argumentation analysis is the recognition and identification of the different forms of argumentative structures in texts. It is a crucial preliminary step for enabling the mining of in-depth argumentative elements in texts. This analysis enables, for example, a researcher to review, evaluate, or validate claims that are found in scientific articles. The difficulty in analyzing argumentation automatically is due to argumentative organization not being easily detected and recognized in texts, nor being well-determined (e.g., correlation with specific word types), nor associated with specific syntactic patterns (e.g., SVO). Understanding argumentation requires deep analysis of texts to identify its organization and logical structure. One type of knowledge that can be used to enable this deep analysis is lexical semantics.Various studies have used recurrent patterns of text orgainzation called *moves* (i.e., text segments that are rhetorical and perform specific communicative goals) to analyze argumentative organization in texts manually [48], or automatically [50]. However, using these patterns with lexical semantic knowledge would provide additional information to more accurately detect and recognize the argumentative elements.

2.1.2 Theoretical Approaches to Argumentation

Swales [48] proposed the Create-A-Research-Space (CARS) model that uses intuition about the argumentative structure of scientific research articles. Swales defined rhetorical moves as text segments that convey communicative goals. He reviewed the Introduction section in 48 articles from social and natural science and found common rhetorical structures among most of these articles. Swales identified three moves in these articles: establishing a research territory, establishing a niche, and occupying the niche. However, despite the widespread influence of the CARS model, some researchers observed two problems: (i) the inconsistent assignment of rhetorical moves to text segments because the identification of the rhetorical moves relies on overall text comprehension, and (ii) a lack of empirical validation of moves in linguistic terms [28].

To overcome these problems, Kanoksilapatham [28] advanced Swales' approach to move analysis by developing a framework that combines his original CARS model with the use of Biber's multidimensional analysis [4] to enrich the model with additional information about linguistic characteristics. Biber's multidimensional analysis [4] is concerned with variation in the speaking and writing of English. Multidimensional analysis can be used to identify differences in linguistic characteristics between various text types at different levels of document structure (e.g., genre, internal section level). Although Kanoksilapatham provides an extension to the Swales' move analysis study, and attempted validation of these moves in biochemistry articles, she only provides a descriptive analysis about rhetorical moves without defining an explicit method for analyzing and recognizing these moves in texts.

Gladkova [19, 20] did a detailed study to identify features that can be linked to argumentative organization in texts. Gladkova's argumentation structures, *topoi*, draw on classical argumentation theory [1]. Gladkova's findings show that argumentative organization is not correlated just by isolated linguistic features but rather with their stylistic *configurations*. The elements of these configurations included lexico-grammatical and semantic relations, syntax, deixis, and coreference. There is a key difference between these well-defined stylistic configurations and the usual loose collections of stylistic features in Machine Learning NLP. Gladkova's features of stylistic configurations interact with one another and with their semantic and syntagmatic environments in rich but regular ways [21]. Although Gladkova's corpus was not annotated by linguists other than herself or by domain experts, since the corpus was small, it would be feasible to include guidelines on how to annotate topoi, as suggested by Cohen et al. [11]

Walton [61] developed a list of argumentation schemes for argumentation analysis. These schemes, forms of argument, aimed to represent common types of arguments including indicative, deductive, and abductive arguments. However, these schemes were not intended for scientific arguments.

Overall, these different approaches based on argumentation theories for analyzing and recognizing argumentative elements, including move analysis ([28] and [48]), argumentative zoning [49], and epistemic topoi [19], lacked a formal knowledge representation which could be used computationally for in-depth argumentation analysis and mining. Another problem in identifying argumentative elements is that few corpora annotated with argumentation structures currently exist for use in training or evaluating Machine Learning classifiers. Thus, this has encouraged researchers to begin developing annotated corpora for use by the Computational Argumentation community ([23] and [24], in particular). In the next section, we will give an overview on some of the state-of-art approaches in computational argumentation including annotation schemes for argumentative texts, extraction of argumentative structures in legal documents, detection of argumentative relations in debate corpus, and others.

2.2 Computational Argumentation

In this section, we describe some of the state-of-the-art approaches in computational argumentation in two main themes: recognizing schemes and detecting argumentation.

2.2.1 Approaches for Recognizing Argumentation Schemes

Argumentative Zoning (AZ) was developed by Teufel and Moens [49] to categorize sentences based on their contextual information (e.g., determining authorship of knowledge claims). The AZ scheme classifies sentences into seven categories including the ones from the CARS model [48]. The data set consisted of 48 computational linguistic papers. Three annotators were involved in the study to extract sentences that fell into these seven categories. The results showed a Kappa score of 83% and 82% between the annotators in the first and second schemes, respectively. The AZ scheme was later modified to suit the characteristics of biology articles [38]. Furthermore, Teufel [51] proposed a revised version of AZ to include more new categorizes for annotating scientific articles such as chemistry. This revised version was planned to model all experimental sciences, which is challenging, since the style of scientific writing varies across disciplines.

Feng and Hirst [16] proposed an approach for recognizing argumentation schemes in the Araucaria corpus [43] that consisted of over 600 manually annotated arguments with their internal structures, premises, and conclusions. These arguments were from various sources including newspapers and court cases. Using the internal structures of arguments identified by the human annotators, the authors developed a method for recognizing the schemes in these arguments and classifying them into their proper categories accordingly. The authors used a set of common argumentation schemes described in [61] which include: argument from example, argument from cause to effect, practical reasoning, argument from consequences, and argument from verbal classification. The authors used statistical classifiers (i.e., one-against-others and pairwise) to classify the arguments into their appropriate schemes. Although, the system achieved accuracies slightly over 90% in classifying annotated arguments in only two of the argumentation schemes, argument from example and practical reasoning, the system performed poorly in classifying other schemes such as argument from consequences and argument from verbal classification.

Liakata et al. [32] developed an annotation scheme called Core Scientific Concepts (CoreSC) to classify sentences into scientific categories (e.g., related to author's other work). The CoreSC scheme consists of three layers: the first includes several categories to classify sentences; the second layer is concerned with properties of these categories; and the third layer creates a link to related instances of the same category. The authors use Machine Learning classifiers (i.e., Conditional Random Fields and Support Vector Machines) to automatically classify sentences into the CoreSC categorizes. The data set consisted of 265 biochemistry and chemistry articles. The authors were only able to achieve an accuracy around 50% in categorizing sentences in the appropriate CoreSC scientific categories which is inadequate for such a task.

Green [23] proposed a plan for creating an annotated corpus of biomedical genetics research articles. Green emphasized that this corpus would be beneficial to the argumentation mining community since it would provide a fine-grained annotation of argumentative components. Also since there are as yet few annotated corpora available, such a corpus would enrich research in the field of Computational Argumentation in general. The author stated that this corpus will be publicly available for further investigation by different research groups in various tasks of argumentation mining.

Green [24] specified a set of argumentation schemes for scientific claims in genetics research articles. The author used a corpus of unannotated genetics research articles, and identified the components (e.g., premises, conclusions) of an argument as well as its type of scheme. Based on the analyses of various genetics research articles, the author specified 10 argumentation schemes that are semantically different. These schemes were new and had not previously been proposed. Furthermore, the specification of argumentation schemes was used to create annotation guidelines. Then, these guidelines were evaluated in a pilot study based on participants' ability to recognize these schemes by reading the guidelines. Overall, the author's ultimate goal for this initial study was to develop annotation guidelines for creating corpora for argumentation mining research. However, based on the pilot study, the results showed a variation in performance since there were two groups of participants (i.e., undergraduate students and researchers). The students performed poorly in recognizing argumentation schemes while the researchers were able to identify these schemes correctly in most cases.

2.2.2 Approaches for Detecting Argumentation

Mochales and Moens [37] proposed a multi-layer approach to detect argumentation in legal texts. These layers included the detection of argumentative information, argument boundaries, relationships between arguments, and the classification of argumentative elements, either as a premise or conclusion. The data set is comprised of legal documents from the European Court of Human Rights (ECHR) corpus. The authors achieved an accuracy of 80% in detecting argumentative units. They also achieved scores between 68% and 74% F1 on the classification of premises and conclusions, respectively. Finally, the last layer detected the argumentation structure by manually parsing the texts using context-free grammar (CFG) rules, achieving an accuracy of 60%.

Cabrio and Villata [8] proposed using a textual entailment approach to detect and identify relationships between arguments in debate discourse. The corpus used in their study was on-line dialogues from Debatepedia, an online resource of arguments on critical issues. Textual entailment infers a directional relation between two text parts. The concept underlying textual entailment is the identification of the correlation, either support or contradiction, between two text segments. For a pair of text segments to be related by entailment, there must be a relation between the segments, termed "Text and Hypothesis", where the initial segment ("Text") is the first part of the argument (entailment) and the second segment ("Hypothesis") is the second part of the argument that either supports or contradicts the first part. In Cabrio and Villata's work, there was no manual identification of the entailment relationships between arguments. However, the authors used Dagan et al.'s [13] approach to defining and detecting textual entailment to infer these relationships. Then the authors identified the accepted arguments using Dung's argumentation theory framework [14]. In this framework, an argument is accepted when all arguments attacking it are rejected. However, an argument would be rejected if one of the attacking arguments is accepted. The result showed an accuracy of 75% in assigning a relation to a pair of arguments which reflects the total number of accepted arguments. However, the data set was too small and included only 200 T-H pairs (i.e., 100 T-H pairs were used to train the system and 100 T-H pairs to test it).

None of these previous approaches to automated argumentation analysis and mining provided a formal knowledge representation that could be used in detecting and recognizing argumentative elements. We believe that developing a formal representational framework based on verb semantics in procedural scientific discourse will enable a more in-depth analysis of argumentative elements in a computationally feasible manner.

Chapter 3

Our Proposed Approach: Argumentative Moves Mirror Scientific Experimental Procedures

3.1 Background

In Section 1.2, we stated our intention to develop a formal knowledge representation based on procedural verbs as a method for argumentation analysis. We also introduced the notion of Swale's CARS model [48] in Section 2.1.2. We hypothesize that recognizing and detecting argumentative moves would provide additional information to our framework of argumentation analysis. We also hypothesize that the Method sections in biochemistry articles contain moves which can be correlated with the author's experimental procedures. These moves can be used to determine salient information about the elements of the article's argumentative structure (e.g., premises) and can contribute to the overall understanding of the author's scientific claims. A key aspect of our hypothesis is that development of a frame-based knowledge representation can be based on the semantics of the verbs associated with these procedures. This representation can provide detailed knowledge for understanding these argumentative moves, which will in turn facilitate analysis of argumentation structure. In other words, we propose that a *procedurally rhetorical verb-centric frame semantics* can be used to obtain a deeper analysis of sentence meaning than is currently the case with simple methods of Information Extraction (e.g., shallow syntactic pattern) and in a computationally feasible manner.

Scientific argument[1] is defined as a process that scientists follow by using certain procedures to obtain empirical data which will either support or defeat their claims, hence leading to the intended conclusion. The strength of a scientific argument depends on its reproducibility and consistency. For a scientific argument to be strong, a scientist should identify and explain all the procedures in their experiment, i.e., reproducibility, so that another researcher who follows the same procedures will reach the same conclusion, i.e., consistency. Thus, for a well-constructed scientific article, a scientist should expect the same conclusion if she follows the same procedures in the same sequence as described in the Method section.

Scientific writing in the biochemistry domain has certain characteristics that made it ideal for our purposes. In this domain, experimental procedures describe the sequence of actions the biochemist performs to carry out an experiment to derive scientific conclusions, to demonstrate science experiments as can be seen in the experimental manuals (e.g., Boyer [5] and Sambrook and Russell [45]). Verbs play an essential role as indicators of these experimental procedures. These procedures can be viewed as corresponding to

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[1] http://www.ces.fau.edu/nasa/introduction/scientific-inquiry/why-do-scientists-argue-and-challenge-each-others-results.php

the elements of the scientific argumentation structure. For example, when examining a biological substance (e.g., a certain type of bacteria) in order to prove a hypothesis (e.g., this bacteria is correlated with a certain disease) the biochemist would perform a sequence of certain procedures to arrive at a conclusion. Essentially, biochemists create an argumentation framework through the scientific methodology they follow—how they perform their experiments is how they argue. We can observe that this genre— biochemistry articles—is procedure-oriented since the scientific procedures that are described are parallel to the scientific argumentation in the text. For example:

Example 1. *"Beads with bound proteins were washed six times (for 10 min under rotation at 4 C) with pulldown buffer and proteins harvested in SDS-sample buffer, separated by SDS-PAGE, and analyzed by autoradiography." [15].*

In this example, the verbs "washed", "harvested", "separated", and "analyzed" are used to illustrate the procedure steps in sequential order. Such an experiment can be reproduced if one follows these steps.

Fillmore [17] introduced the notion of frame semantics as a theory of meaning. A *semantic frame* is defined as "any coherent individuatable perception, memory, experience, action or object" by Fillmore [18]. In other words, coherently structured concepts that are related to each other to represent a complete knowledge of world events or experiences. For example, to understand the word "buy", one would access the knowledge contained in the commercial transaction frame which includes words such as the person who buys the goods (buyer), the goods that are being sold (goods), the person who sells the goods (seller), and the currency that the buyer and seller agree on (money).

Following Fillmore's theory of frame semantics, FrameNet [2] was developed to create an online lexical resource for English. This framework includes more than 170,000 manually annotated sentences and 10,000 words. The computational linguistic community has been attracted to the concept of the frame semantics and developed computational resources using this concept, such as VerbNet [47], an on-line verb lexicon for English and PropBank [40], an annotated corpus with basic semantic propositions.

Following the notion of frame semantics, we propose to build a knowledge representation framework to analyze verbs in a procedural-oriented genre. Our concept of procedurally rhetorical verb-centric frame semantics is intended to address this gap by developing a computationally feasible knowledge representation that will enable argumentation analysis. The knowledge contained in the frame semantics will facilitate the extraction of elements of arguments, i.e., argumentation mining. To reiterate, our hypothesis is that procedurally rhetorical verb-centric frame semantics can provide a knowledge representation framework for analyzing and representing the meanings of the verbs used in biochemistry articles. In turn, these frames will facilitate the identification of argumentation structure in the discourse describing experimental procedures.

3.2 The Experimental Event

We have developed a new annotation scheme based on the concept, *experimental event*, for identifying the structured representation of knowledge in a set of sentences describing the experimental procedures in the Method sections of biochemical articles. Several researchers have developed other forms of schemes (e.g., "bio-events", [54]) to extract biological information (e.g., gene regulation). However, a bio-event is different from our definition of an experimental event. On the one hand, a bio-event is concerned with detection of bio-molecular events within the biomedical literature, such as the identification of events that are related to given proteins [54]. In our case, an experimental event is concerned with processes and procedures that are used to investigate biological events. The experimental event is also concerned with the recognition of the biochemist's reasoning of standard biochemical procedures such as using certain instruments or specific biological materials.

Our annotation scheme was inspired by the annotation scheme for bio-events occurring in biomedical articles, which was developed by the National Center for Text Mining (NaCTeM) [55]. We adapted and modified the bio-event annotation scheme and also added new semantic roles to define our experimental event. Our experimental event scheme includes: *move type*, *move trigger*, *event trigger*, *event theme*, *event cause*, *repetition of process*, *process time*, *process temperature*, *process condition*, and *instrument type*. The move type plays a central role among all semantic roles in the experimental event because it is concerned with the identification of rhetorical moves in the biochemical texts, so we will describe this semantic role first. Then, the definition of the remaining roles will be presented in Table 3.1.

Move type: This feature is concerned with the classification of various argumentative moves found in texts. We have developed a new model for these argumentative moves inspired by the work of Kanoksilapatham [28, 29]. That is, we have adapted and modified some of Kanoksilapatham's argumentative moves, as well as adding new more fine-grained argumentative moves to our model. In combination, there are four major argumentative moves concerned with the method sections in biochemistry articles as can be seen in Table 3.1.

In addition, Table 3.2 shows the remaining semantic roles in the annotation scheme of our experimental event. In order to understand how each one of these semantic roles is used, we show an example in detecting these semantic roles manually from our data set. In this case, we will use the aforementioned Example 1 as follows. Table 3.3 shows the

Table 3.1: Argumentative Moves in the Method Sections of Biochemistry Articles

Move type	Definition
Description-of-method	Concerned with sentences that describe experimental events.
Appeal-to-authority	Concerned with sentences that discuss the use of well-established methods.
Background information	Concerned with all background information for the experimental events such as “method justification, comment, or observation, exclusion of data, approval of use of human tissue” as defined by Kanoksilapatham (2003).
Source-of-materials	Concerned with the use of certain biological materials in the experimental events.

result of assigning various text segments in Example 1 to semantic roles. As seen in Table 3.3, we have manually assigned text segment(s) to a particular semantic role based on their correlation. For example, we identify the move type as a description of the method because of the subsequent use of procedural verbs (e.g., *washed* and *harvested*) which convey a sequence of actions. So, these verbs triggered this move type (i.e., the reason for assigning these verbs include: *washed*, *harvested*, *separated*, and *analyzed* to the semantic role, move trigger). These aforementioned verbs are also assigned to the semantic role, event trigger, because these words evoked various events (e.g., harvesting and separating of proteins). The assignments of other semantic roles are straightforward as seen in Table 3.3. In the previous example, we have detected these semantic roles manually. However, we aim to recognize and detect these semantic roles automatically using Machine Learning methods to accurately assign text segments to the appropriate semantic role. Our goal

Table 3.2: Semantic Roles in the Annotation Scheme of our Experimental Event

Semantic role	Definition
Move trigger	Concerned with word(s) or phrase(s) in the sentence(s) that identify the type of argumentative move. A move trigger could be a sequence of words (verbs) or a phrase.
Event trigger	"A word or phrase around which the event is organized in the text" as defined by Thompson et al. (2011). The trigger could be a verb such as *compare*, or a nominalized verb such as *transcription* or *activation*.
Event theme	An item or participant that has been affected during the event.
Event cause	An item or participant that is responsible for the event to occur.
Repetition of process	Identifies the frequency of a process to be performed.
Process time	Concerned with the duration that a process takes to be completed.
Process temperature	The temperature of a performed process.
Process condition	Describes the method by which an experimental event has been carried out (e.g., under rotation, stirring, agitation, sonication).
Instrument type	Identifies the type of instrument(s) used in the experimental event.

Table 3.3: Detection of our Semantic Roles in Example 1

Semantic role	Assigned text segment
Move type	**Description of method**
Move trigger	*washed*, *harvested*, *separated*, *analyzed*
Event trigger	*washed*, *harvested*, *separated*, *analyzed*
Event theme	*Beads with bound proteins*
Event cause	*pulldown buffer*, *SDS-sample buffer*, *SDS-PAGE*, *autoradiography*
Repetition of process	*six times*
Process time	*10 min*
Process temperature	*4 C*
Process condition	*under rotation*
Instrument type	*pulldown buffer*, *SDS-sample buffer*, *SDS-PAGE* , *autoradiography*

is to build upon these semantic roles a higher level of abstraction that contains a richer knowledge representation of this genre.

Chapter 4

Our Proposed Methodology

4.1 Introduction

We have created a data set consisting of 105 text files. These files include only the Method sections from biochemistry journal articles which were randomly selected from PubMed Central (PMC). To prepare the data set for our task, all files were converted to plain text files that included one sentence per line and all figures and tables were omitted from these files. We also applied some annotation methods to the data set such as part-of-speech (POS) tagging (i.e., GENIA Tagger[1]) and sentence parsing (i.e., BLLIP Parser[2]).

We are proposing to develop a knowledge representation framework based on procedurally rhetorical verb-centric frame semantics to analyze and recognize argumentation in biochemical texts. To do this, we will use the following methodology as follows in the upcoming sections respectively.

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[1] http://www.nactem.ac.uk/GENIA/tagger/

[2] http://bllip.cs.brown.edu/resources.shtml

4.2 First Step: Annotation and Guidelines

Wattarujeekrit et al. [62] developed guidelines for annotating Predicate-Argument Structure (PAS) in molecular biology articles following the PropBank annotation guidelines [30]. However, Wattarujeekrit et al. focused only on verbs that describe molecular events in biology. Tsai et al., [57] developed a training dataset using Wattarujeekrit et al.'s guidelines to train a Machine Learning model to automatically label and classify verb arguments in PAS with the proper semantic roles. In this research, we will develop guidelines to annotate semantic roles, verb arguments in PAS, and argumentative moves. We will be using Tsai et al.'s [57] guidelines as an example to create our own guidelines for annotating semantic roles. We will also be using Teufel's [51] and Kanoksilapatham's [28] annotation guidelines as a model to create our guidelines for annotating argumentative moves. Teufel's annotation guidelines are based on binary decision trees that allow the annotators to select and associate text segments with their proper categories. However, Teufel's guidelines are designed for different genres (e.g., Computer Science and Chemistry articles). Kanoksilapatham's guidelines are designed for biochemistry articles, which this research focuses on. Nevertheless, Kanoksilapatham [28] only provided a brief summary of the guidelines in her thesis. The manual annotation tasks will be performed by two biochemist annotators who will be trained using our annotation guidelines. To facilitate the annotation tasks, annotators will be using software (e.g., WordFreak[3]) to add, modify, and save their annotation in files. In the following example, we show how semantic roles will be manually annotated using our annotation guidelines. For example:

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[3] http://wordfreak.sourceforge.net/

Example 2. *"Beads with bound proteins [Theme] were washed [predicate] six times [Repetition of process] (for 10 min [Process time] under rotation [Process condition] at 4 C [Process temperature]) with pulldown buffer [Cause] and proteins [Theme] harvested [predicate] in SDS-sample buffer [Cause], separated [predicate] by SDS-PAGE [Cause], and analyzed [predicate] by autoradiography [Cause]." [15].*

4.3 Second Step: Labelling Semantic Roles

The dataset will be manually annotated using the guidelines for semantic roles which will be developed in the first step. Then, the manually annotated dataset will be used to train a Machine Learning model. Semantic Role Labeling (SRL) was developed by Tsai et al. [56] to automatically label words with their proper semantic roles. SRL was used with the biomedical corpus in [57] to improve the biomedical relation-extraction system for identifying additional information in complex biological relations (e.g., location and manner). The results showed that SRL achieved an F1 score between 84% and 86% [57, 58]. SRL uses supervised Machine Learning methods including Support Vector Machines (SVMs) and Maximal Entropy (ME) to classify the types of arguments from the parsed trees of a dataset. Since we will be using the BLLIP parser which has been trained on biomedical and newswire corpora, the SRL system then will be evaluated using a new data set with its parsed trees, which will be produced by the BLLIP parser. However, the BLLIP parser fails sometimes when it parses sentences that contain complex biological text segments (e.g., "5'GATGACAGGGAAGCTGGA"). So, we will filter these types of complex text segments from sentences before the parsing trees are constructed by the BLLIP parser. Since we will be using the SRL system to automatically annotate semantic roles in sentences, the annotation produced will be considered as a silver standard [44] because it is a machine-based annotation.

4.4 Third Step: Creating Procedurally Rhetorical Frame Semantics

We will be also using FrameNet [2] and VerbNet [47] as models to create rhetorically procedural frame semantics. Essentially, FrameNet frames are based on scenes and VerbNet frames are based on verbs. FrameNet and VerbNet resources will be the grounds to create our frames. We may find out that Method sections in biochemistry articles use certain verbs more frequently than others. In the following example, we show how different semantic frames are presented for the verb "incubate".

Example 3. *"Cells were incubated with the DNA in serum-free DEAE-dextran/MEM media overnight." [3].*

Example 4. *"Cells were incubated at room temperature with 3% or 12% PFA for 30 or 60 minutes in PBS, quenched with 100 mM ammonium chloride, washed in PBS, lysed on ice and snap frozen in liquid nitrogen." [7].*

Example 5. *"Chambers were incubated for 18 hours after which time the number of cells in the lower chamber was determined." [36].*

4.5 Fourth Step: Detecting Argumentative Moves

After the automatic labelling for semantic roles in our dataset using the SRL model in Section 4.3, we will annotate argumentative moves in the data set using the guidelines for annotating argumentative moves. Then, this dataset will be used to train a new Machine Learning model that uses supervised Machine Learning methods (e.g., SVMs and Decision Trees) that we will develop to classify sentences into different argumentative move categories. We will be using the semantic roles derived from SRL as features to train the machine learning model for detecting argumentative moves. We should also note that these features come from an automatic system which only delivers up to 86% of correct semantic role labeling [57, 58]. Various features will be used in the machine learning model such as the semantic roles (event manner, event location) that are likely to be associated with each argumentative move.

4.6 Fifth Step: Evaluation

We will perform two evaluation steps for the SRL model and the model for detecting argumentative moves. We will use precision, recall, and F1 score calculations to measure the performance of the SRL model. Then, we will use the information from the annotated argumentative moves from the first step as the gold standard as well as precision, recall, and F1 score calculations to evaluate the argumentative moves derived from our machine learning model.

Chapter 5

Semantic Roles: Towards Rhetorical Moves in Writing About Experimental Procedures

5.1 Introduction

Scientists must routinely review the scholarly literature in their fields to keep abreast of current advances and to retrieve information relevant to their research. However, this undertaking is becoming more difficult as the volume of scientific literature is immense and rapidly increasing. The types of tasks currently handled by Biomedical Natural Language Processing (BioNLP) systems have generally been aimed at extracting very specific and limited information, for example, protein and gene names and relations [12], and so have been able to rely on relatively simple forms of information extraction. Although these approaches fulfil some information needs, more in-depth and comprehensive information contained in biomedical texts would be highly valuable to scientists. This type of information can enable validating scientific claims, tracing current research directions, reproducing scientific procedures, and so forth. Recently, a new and more challenging information extraction task has been introduced as a means of obtaining this type of information: identifying the argumentation structure in biomedical articles (e.g., [23] and [24]).

The essence of argumentation can be considered as influencing others to gain their adherence to a particular idea [41]. Arguments have an explicit logical structure, for example, claims that are backed with reasons, which in turn are supported by evidence, leading to conclusions [53]. Argumentation analysis is the recognition and identification of the different forms of argumentative structures in texts. Various studies have used recurrent patterns of text organization called *rhetorical moves* (i.e., text segments that are rhetorical and perform specific communicative goals) to analyze argumentative organization of texts manually [48] or automatically [50]. Swales' CARS model targets the Introduction section[1] of scientific articles. Teufel's interests are concentrated on rhetorical moves associated with defining the research space and suggesting the knowledge claims for computational linguistics and chemistry articles. Kanoksilapatham adds to these works by providing the first comprehensive set of rhetorical moves for complete biochemistry articles [28].

With our long-term goal being analyzing argumentation in biochemistry articles, our mid-term research goal is to provide a computational model for Kanoksilapatham's descriptive rhetorical move taxonomy. Initially, our focus is on the Methods section of the taxonomy since this provides a description of the procedures followed in the experiment and the analysis of the results of the experiment thereby giving a framework for analyzing the

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[1] Experimental articles in the biomedical sciences normally organized in the IMRaD style: Introduction, Methods, Results, and Discussion.

moves in the remainder of the article. Because the experimental process is procedural, the moves tend to follow the verbs describing the steps in the experimental process. In other words, argumentation structure and scientific method both consist of rhetorical moves and experimental process, respectively. When a scientist describes her/his method in the writing, it contains a list of experimental steps which are described by verbs (actions). These verbs evoke (initiate) the rhetorical moves in the writing. To understand the moves, we need information about the semantic roles associated with these procedural verbs. Two well known databases containing semantic role information, Framenet [2] and Verbnet [47], do not provide the information appropriate for the verbs found in this scientific domain. So, our purpose in this paper, in the spirit of these two databases, is to introduce the semantic roles that we are proposing for this domain, some of which are the same as those normally found and some which are new and we suggest are required for this domain.

The structure of the document will be as follows: First, an overview of some theoretical and computational approaches to argumentation are presented in Section 5.2. Then, our proposed approach to argumentation analysis is described in Section 5.3. Next, a description of our annotation scheme is given in Section 5.4. Finally, the future work and a conclusion of this paper is given in Section **??**.

5.2 Related Work

Over the past decade, the focus on argumentation mining has been growing significantly in different areas of Artificial Intelligence (AI) research. The incentive to build Natural Language Processing (NLP) systems to automatically identify and analyze argumentative components in various genres of texts has increased because knowledge of argumentative structure facilitates various tasks such as text summarization [50]. Various computational studies have been done to analyze different argumentation aspects, including: the structure of valid arguments in scientific articles ([22], [23] and [24]). In particular, researchers are developing automated argumentation analysis systems to enable scientists in the experimental sciences to review and evaluate scientific findings more efficiently, and to help identify whether scientific claims are valid or not, based on their argumentative structure (e.g., [32] and [51]).

Swales [48] proposed the Create-A-Research-Space (CARS) model that uses intuition about the argumentative structure of scientific research articles. Swales identified three moves in these articles: establishing a research territory, establishing a niche, and occupying the niche. However, despite the widespread influence of the CARS model, some researchers observed two problems: (i) the inconsistent assignment of rhetorical moves to text segments because the identification of the rhetorical moves relies on overall text comprehension, and (ii) a lack of empirical validation of moves in linguistic terms [28].

To overcome these problems, Kanoksilapatham [28] advanced Swales' approach to move analysis by developing a framework that combines his original CARS model with the use of Biber's multidimensional analysis [4] to enrich the model with additional information about linguistic characteristics. Although Kanoksilapatham provides an extension to the Swales' move analysis study and attempted validation of these moves in biochemistry articles, she only provides a descriptive analysis about rhetorical moves without defining an explicit method for analyzing and recognizing these moves in texts.

Argumentative Zoning (AZ) was developed by Teufel and Moens [49] to categorize sentences based on their contextual information (e.g., determining authorship of knowledge claims). The AZ scheme was later modified to suit the characteristics of biology articles [38]. Furthermore, Teufel [51] proposed a revised version of AZ to include more new categorizes for annotating scientific articles such as chemistry. Green [23] proposed a plan for creating an annotated corpus of biomedical genetics research articles suitable for analyzing argumentation.

Overall, these different approaches based on argumentation theories for analyzing and recognizing argumentative elements, including move analysis ([28] and [48]) and argumentative zoning [49] lack a formal knowledge representation which could be used computationally. When focusing on procedural verbs, as we are suggesting here, semantic roles can provide an important aspect of this needed knowledge. The FrameNet project [2], an online lexical database for English, provides semantic roles for verbs in ordinary English and links to a large number of semantic frames. BioFrameNet [**?**] is a domain specific extension to FrameNet for molecular biology, in particular. VerbNet [47] is also an on-line verb lexicon for ordinary English containing semantic roles and frames.

We believe that developing a formal representational framework based on verb semantics in procedural scientific discourse will enable a more in-depth analysis in a computationally feasible manner.

5.3 Our Proposed Approach: Rhetorical Moves Mirror Scientific Experimental Procedures

We aim to develop a formal knowledge representation based on procedural verbs as a method for rhetorical move analysis. We have introduced the notion of moves [48] [28] in Section 2. We also hypothesize that the Method sections in biochemistry articles contain moves which can be correlated with the author's experimental procedures. A key aspect of our hypothesis is that development of a frame-based knowledge representation can be based on the semantics of the verbs associated with these procedures. This representation can provide detailed knowledge for understanding these rhetorical moves, which will in turn facilitate analysis of argumentation structure. In other words, we propose that a *procedurally rhetorical verb-centric frame semantics* can be used to obtain a deeper analysis of sentence meaning in a computationally feasible manner.

Scientific writing in the biochemistry domain has certain characteristics that make it ideal for our purposes. In this domain, experimental procedures describe the sequence of actions the biochemist performs to carry out an experiment to derive scientific conclusions, to demonstrate science experiments as can be seen in the experimental manuals (e.g., [5] and [45]). Verbs play an essential role as indicators of these experimental procedures. These procedures can be viewed as corresponding to the elements of the scientific argumentation structure. For example, when examining a biological substance (e.g., a certain type of bacteria) in order to prove a hypothesis (e.g., this bacteria is correlated with a certain disease) the biochemist would perform a sequence of certain procedures to arrive at a conclusion. Essentially, biochemists create an argumentation framework through the scientific methodology they follow—how they perform their experiments is how they argue. We can observe that this genre—biochemistry articles—is procedure-oriented since the scientific procedures that are described are parallel to the scientific argumentation in the text. For example:

Example 6. *"Beads with bound proteins were washed six times (for 10 min under rotation at 4 C) with pulldown buffer and proteins harvested in SDS-sample buffer, separated by SDS-PAGE, and analyzed by autoradiography." [15].*

In this example, the verbs "washed", "harvested", "separated", and "analyzed" are used to illustrate the procedure steps in sequential order. Such an experiment can be reproduced if one follows these steps.

Fillmore [17] introduced the notion of frame semantics as a theory of meaning. A *semantic frame* is defined by Fillmore as “any coherent individuatable perception, memory, experience, action or object” [18]. In other words, coherently structured concepts that are related to each other to represent a complete knowledge of world events or experiences. For example, to understand the word “buy”, one would access the knowledge contained in the commercial transaction frame which includes words such as the person who buys the goods (buyer), the goods that are being sold (goods), the person who sells the goods (seller), and the currency that the buyer and seller agree on (money).

Following Fillmore’s theory of frame semantics, FrameNet [2] was developed to create an online lexical resource for English. This framework includes more than 170,000 manually annotated sentences and 10,000 words. The computational linguistic community has been attracted to the concept of the frame semantics and developed computational resources using this concept, such as VerbNet [47], an on-line verb lexicon for English and PropBank [40], an annotated corpus with basic semantic propositions.

Following the notion of frame semantics, we propose to build a knowledge representation framework to analyze verbs in a procedurally-oriented genre. Our concept of verb-centric frame semantics is intended to address this gap by developing a computationally feasible knowledge representation that will enable the analysis of rhetorical moves.

5.4 Experimental Event Annotation Scheme

We have developed a new annotation scheme for identifying the structured representation of knowledge in a set of sentences describing the experimental procedures in the Method sections of biochemical articles. Several researchers have developed other forms of schemes (e.g., “bio-events”, [54]) to extract biological information (e.g., gene regulation). However, a bio-event is different from our definition of an experimental event. On the one hand, a bio-event is concerned with detection of bio-molecular events within the biomedical literature, such as the identification of events that are related to given proteins [54]. In our case, an experimental event is concerned with processes and procedures that are used to investigate biological events. The experimental event is also concerned with the recognition of the biochemist's reasoning of standard biochemical procedures such as using certain instruments or specific biological materials.

Our experimental event scheme was inspired by the annotation scheme for bio-events occurring in biomedical articles, which was developed by the National Center for Text Mining (NaCTeM) [55]. We based our experimental event scheme on the inventory of semantic roles in VerbNet [47] and modified and added new semantic roles to define our scheme. Our experimental event scheme includes: *Theme*, *Patient*, *Predicate*, *Agent*, *Location*, *Goal*, etc. The complete set of semantic roles and their definitions in our experimental event scheme is presented in Table 5.1.

We have extended the VerbNet definition of the semantic role *Instrument* from simply describing "an object or force that comes in contact with an object and causes some change in them" [47] to include a variety of subcategories that correspond to various types of biological and man-made instruments that are used in a biochemistry laboratory. These subcategories include:

1- Instruments used to *change* the state of an object. For example:

Example 7. *"Beads with bound proteins were washed six times (for 10 min under rotation at 4 C) with **pulldown buffer** ..." [15].*

In this example, the pulldown buffer was used to wash (change the state of) the Beads with bound proteins. In this instance, the phrase "pulldown buffer" should be labeled as

instrument (change).

2- Instruments used to *maintain* the state of an object. For example:

Example 8. *"Once the samples were in EPR tubes, they were immediately frozen in liquid nitrogen, and stored in* ***liquid nitrogen*** *before using." [**?**].*

In this example, the liquid nitrogen was used to store (maintain the condition of) the samples which were in the EPR tubes. In this case, the phrase "liquid nitrogen" should be labeled as **instrument (maintain)**.

3- Instruments used to *observe* an object. For example:

Example 9. *The mitochondria was observed by* ***spinning disk confocal microscopy****.*

The spinning disk confocal microscopy is used to observe the mitochondria. We should label the phrase "spinning disk confocal microscopy" as **instrument (observe)**.

4- Instruments used as a *catalyst* in experimental processes to occur. For example:

Example 10. *"The ca. 900 bp PCR products were digested with* ***NdeI and HindIII*** *and ligated into pUC19." [**?**].*

In this example, the NdeI and HindIII are enzymes used to facilitate the digestion (cutting) of the ca.(approximately) 900 bp PCR products. In this instance, the phrase "NdeI and HindIII" should be labeled as **instrument (catalyst)**.

5- Instrument used to *measure* an object. For example:

Example 11. *"Beads with bound proteins were washed six times (for 10 min under rotation at 4 C) with pulldown buffer and proteins harvested in SDS-sample buffer, separated by SDS-PAGE, and analyzed by* ***autoradiography****." [15].*

In this example, the autoradiography was used to analyze (measure) the proteins. In this example, the word "autoradiography" should be labeled as **instrument (measure)**.
6- It could be used to describe a *mathematical or computational instrument* (e.g., simulation, algorithm, equation, and the use of software). For example:

Example 12. *"Simulations of these EPR spectra were accomplished with* ***the computer program QPOWA [30,31])****." [?].*

The computer program QPOWA was used here as computational instrument to perform simulations of the mentioned above EPR spectra. So, the phrase "the computer program QPOWA [30,31]" should be labeled as **instrument (computational instrument)**.
7- Finally it could be used as a *reference* for method or protocol that being used. For example:

Example 13. *"The preparation of authentic vaccinia H5R protein and recombinant B1R protein kinase were* ***as previously described [11]****." [6]*

The phrase "as previously described [11]" is to indicate that the authors referring to other method that they used in their current experimental process. We should label the phrase "as previously described [11]" as **instrument (reference)**. These sub-categories of the semantic role (instrument) are not exclusive to the mentioned types above. However, based on our full-text analysis, these instrument types are most comprehensive ones. We will add or update these sub-categories if we encountered a new type (usage) of instrument.

We have also proposed a new semantic role *protocol detail* that identifies certain types of information about experimental processes which include:
1- Time or the duration of a process [47]. For example:

Example 14. *“Beads with bound proteins were washed six times (**for 10 min** under rotation at 4 C) with pulldown buffer ...” [15].*

2- Temperature of an experimental process. For example:

Example 15. *“Beads with bound proteins were washed six times (for 10 min under rotation **at 4 C**) with pulldown buffer ...” [15].*

3- Condition or manner of which an experimental process was carried out. For example:

Example 16. *“Beads with bound proteins were washed six times (for 10 min **under rotation** at 4 C) with pulldown buffer ...” [15].*

4- Buffer which is “a solution containing either a weak acid and a conjugate base or a weak base and a conjugate acid, used to stabilize the pH of a liquid upon dilution.” [2] For example:

Example 17. *“For phosphorylation, three identical reactions contained H5R protein (70 pmol), B1R protein kinase (90 μl), **Tris-HCl, pH 7.4 (20 mM)**, magnesium chloride (5 mM), ATP (50 μM), [Î-32P] ATP (50 μCi) and dithiothreitol (2 mM) in a total volume of 500 μl.” [6].*

5- Cofactor is defined as “inorganic substances that are required for, or increase the rate of, catalysis.”[3] For example:

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[2] Buffer - Biology-Online Dictionary. (n.d.). Retrieved September 23, 2017, from http://www.biologyonline.org/dictionary/Buffer

[3] coenzymes and cofactors. (n.d.). Retrieved September 23, 2017, from http://academic.brooklyn.cuny.edu/biology/bio4fv/page/coenzy_.htm

Example 18. *"For phosphorylation, three identical reactions contained H5R protein (70 pmol), B1R protein kinase (90 μl), Tris-HCl, pH 7.4 (20 mM),* ***magnesium chloride (5 mM), ATP (50 μM), [Î-32P] ATP (50 μCi) and dithiothreitol (2 mM)*** *in a total volume of 500 μl."* [6].

6- Repetition of a step in experimental processes. For example:

Example 19. *"Beads with bound proteins were washed* ***six times*** *(for 10 min under rotation at 4 C) with pulldown buffer ..."* [15].

5.5 Manual Analysis

We now present some of the manual analysis of the Method section from three articles from our corpus based on our semantic roles given in the previous section. Table 5.2 shows some sentences from these articles. The purpose of this analysis is to identify the semantic roles of experimental processes and the semantic frames of procedural verbs that occurred in these processes. The sentences in Table 5.2 discussed the idea of cutting a DNA piece of a plasmid, which is "a small circular and double-stranded DNA molecule that is distinct from a cell's chromosomal DNA"[10], and ligate (attach) that piece to new plasmid to produce the desired protein. Table 5.3 showed five actual events from the sentences in Table 5.2. The events 1, 2, 3, and 4 are extracted from the sentence no.1 and the sentence no.2 has only event 5, while there is no actual experimental event in sentence no.3 rather simply

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[9] http://verbs.colorado.edu/ mpalmer/projects/verbnet.html

[9] http://www.glossary.sil.org/term/factitive-semantic-role

[10] plasmid / plasmids — Learn Science at Scitable. (n.d.). Retrieved December 22, 2017, from https://www.nature.com/scitable/definition/plasmid-plasmids-28

Semantic role	Definition
Agent	“Generally a human or an animate subject. Used mostly as a volitional agent, but also used in VerbNet for internally controlled subjects such as forces and machines”[4].
Patient	“used for participants that are undergoing a process or that have been affected in some way”[5].
Predicate	A word that initiates the frame. It could be a verb such as *compare*, or a nominalized verb such as *transcription* or *activation*.
Theme	“used for participants in a location or undergoing a change of location”[6].
Goal	Identifies a thing toward which an action is directed or place to which something moves [7].
Factitive	“An referent that results from the action or state identified by a verb” [8].
Location	The physical place where the experiments took place.
Protocol-Detail:Time	Identifies the time or a duration of an experimental process.
Protocol-Detail:Temperature	Identifies the temperature of an experimental process.
Protocol-Detail:Condition	Identifies the condition of how an experimental process being carried out (e.g., under rotation).
Protocol-Detail:Repetition	Identifies the number of times that an experimental process being repeated.
Protocol-Detail:Buffer	Identifies the buffer that was used in an experimental process.
Protocol-Detail:Cofactor	Identifies the cofactor that was used in an experimental process.
Instrument:Change	In general, instrument “used to describe objects (or forces) that come in contact with an object and cause some change in them” VerbNet project[9]. So, Instrument: (Change) describe an object or protocol that can change another object(s).
Instrument:Measure	Describes an object or protocol that can measure another ob-

referring to a section in the original article. Each event in Table 5.3 contain one complete thought (a clause), which means there is at least one predicate and one subject. Also the actual sequence of experimental events in the lab don't necessarily follow the sequence that these events appeared in the texts. Another important aspect to note is that not all the essential information about experimental processes is found in the text, some information can be implied. However, these implied pieces of information can be inferred from the ontology of standard biochemistry procedures, which is not yet available. For example, let us take a look in Table 5.3 for the events (1 to 4):

1- Digestion of pUB5832 - so the relevant piece (900 bp piece) was cut out using two restricted enzymes (NdeI and HindIII)

2- Then, the purification of 900 bp piece - gel electrophoresis was used in this purification step which is an implied information

3- Then at any time, the digestion of puc19 happens,

4- Before the ligation of 900 bp into puc19 occurred.

So, by reading the description of events in sentence no.1, one can not fully comprehend the sequence of the events nor the events themselves without the knowledge of what are the involved aspects in performing a plasmid digestion, purification, and ligation.

Our experience with annotating the biochemistry articles with our expert, we recognized that not all of the information needed to interpret the move structure is available in the text. What is needed is an ontology that captures the knowledge that a working biochemist would have regarding biochemistry experimental procedures, especially the sequence of events that are normally undertaken in these laboratory procedures. We build such an ontology and the following section will describe it in more detail.

No.	Sentence
1	The over-expression plasmid for L1, pUB5832, was digested with *Nde*I and *Hind*III, and the resulting ca. 900 bp piece was gel purified and ligated using T4 ligase into pUC19, which was also digested with *Nde*I and *Hind*III, to yield the cloning plasmid pL1PUC19.
2	Mutations were introduced into the L1 gene by using the overlap extension method of Ho et al. [60], as described previously [68].
3	The oligonucleotides used for the preparation of the mutants are shown in Table1.1.

Table 5.2: Some sentences from the article **Biochem-3-_-77373** [?]

Event 1	Event 2	Event 3
• Patient: The over-expression plasmid for L1, pUB5832 • Predicate: digested • Instrument (catalyst): NdeI and HindIII	• Patient: the resulting ca. 900 bp piece • Predicate: gel purified • Instrument (catalyst): Gel electrophoresis	• Patient: pUC19 • Predicate: digested • Instrument (catalyst): NdeI and HindIII

Event 4	Event 5	Event 6
• Patient: the resulting ca. 900 bp piece • Predicate: ligated • Instrument (catalyst): using T4 ligase • goal: into pUC19	• Patient: the L1 gene • Predicate: introduced (mutated) • Instrument (reference type): using the overlap extension method of Ho et al.	Sentence no.3 doesn't contain any experimental event.

Table 5.3: Extracted events from some sentences from the article **Biochem-3-_-77373** [?]

Example	Syntactic frame	Semantic frame
“Beads with bound proteins were washed six times (for 10 min under rotation at 4 C) with pulldown buffer ...” [15].	NP V PP PP PP PP	Patient Protocol-Detail (Repetition, Time, Condition, Temperature) Instrument (Change)
“The gels were finally washed with 0.1 M Tris-HCI buffer”.	NP V PP	Patient Instrument (Change)

Table 5.4: Semantic frames for the verb *wash*

Chapter 6

Biochemistry Procedure-Oriented Ontology

6.1 Introduction

Ontologies provide entities (known as individuals in some ontological languages) and concepts, and relations among those entities and concepts. Ontologies must provide relations that are required by the domain being represented. Our interest is centred on the biochemistry domain, the experimental methodology aspect, in particular.

A number of biologically oriented ontologies have been created, one of the best known is the Gene Ontology (GO) [**?**]. Others have been developed for a variety of other purposes. They are discussed in detail in the next section. Most of these ontologies describe a set of concepts and categories in the biological domain that shows their properties and the relations between them.

The type of domain that we are attempting to represent consists of *procedures*, experimental procedures, in particular. Procedures are *sequences* of *procedure steps* (simply, *steps*, henceforth). Some ontologies provide descriptions of steps [**?**]. To the best of our knowledge no current biologically oriented ontology represents sequences of steps. An important aspect of the steps in a procedure is that they immediately follow one another. 'Immediately follows' (and 'immediately precedes') is an intransitive relation (i.e., if B immediately follows A, and if C immediately follow B, then C does not immediately follow A). Transitive relations are the norm in the current biologically oriented ontologies (e.g., the omnipresent 'subclass' relation; 'proper part of', 'precedes' and 'is causally related to' ([**?**], Figures 6 and 9)).

Procedures can contain sequences of steps that are totally ordered (i.e., the steps must be done one after the other in the sequence specified), steps that can be partially ordered (i.e., subsequences of steps that can be done in any order), and alternative subsequences of steps (i.e., only one of the alternatives is done). In addition to the intransitive relations 'immediately follows' and 'immediately precedes' our contribution also includes these three types of sequence orderings.

The scientific domain of interest to us is biochemistry. Standard experimental procedures, which typically involve several steps, are described in detail in manuals of standard biochemical procedures [**?**, **?**]. We are developing a framework for biochemistry procedure-oriented ontologies to explicitly identify all of the steps of an experimental procedure and to provide the relations between these steps. An example of an ontology following this framework is described in this paper. This case study investigates one experimental procedure, Alkaline Agarose Gel Electrophoresis, that exists in the manual of standard biochemical procedures.

6.2 Related Work

Developing ontologies has become increasingly crucial in the biomedical domain in general [?]. Several ontologies have been developed in recent years such as the Gene Ontology [?], the Ontology for Chemical Entities of Biological Interest (ChEBI) [?], the Ontology for Biomedical Investigations (OBI) [?], and the Foundational Model of Anatomy (FMA) [?]. Mainly, the goal of these ontologies is to provide definitive controlled terminologies that describe entities in the biomedical genre.

The main aspect of Gene Ontology (GO) is to provide information that describes gene products using precisely defined vocabulary [?]. GO intially used three model organism databases including FlyBase [?], Mouse Genome Informatics [?, ?], and the saccharomyces Genome Database [?]. Recently, the number of model organism databases has increased dramatically [?].

The Chemical Entities of Biological Interest ontology (ChEBI) is a lexicon of molecular entities that is concerned with small molecules [?]. Data from several resources (e.g., IntEnz [?], KEGG COMPOUND [?], and the Chemical Ontology) were used in the creation of ChEBI. ChEBI used various relations to describe the relationships between ontology entities. These relations include relations required by ChEBI (e.g., 'is conjugate acid of', and 'is tautomer of') as well as relations which are defined by the Relations Ontology [1] (e.g., 'is a' and 'is part of').

The Ontology for Biomedical Investigations (OBI), `http://purl.obolibrary.org/obo/obi`, [?], is a resource for annotating biomedical investigations. This ontology provides the standard tools to represent study design, protocols and instrumentation used, the data generated and the types of analysis performed on the data. A number of ontologies [?],

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[1] http://www.obofoundry.org/ontology/ro.html

[?], [?], [?], [?] have been based on the OBI ontology. These ontologies are closest to our interest in biochemistry procedures.

A work that predates the above list, [?], proposes EXPO, an ontology of scientific experiments, in general. It remains a descriptive ontology, providing a detailed description of the various aspects of scientific experiments and how they are related.

Descriptions of experimental processes are provided by OBI, and three real-world applications are discussed in [?]. Some of the relations in these applications (e.g., inputs, outputs, etc.) come very close to our purpose here. The beta cell genomics application ontology (BCGO) [?] also uses OBI, but it tends to be a more descriptive ontology than some of the others that use OBI, but some of the relations in RO, the relation ontology [?], that are used (e.g., produces, translate_to) do have an ordering sense.

The two ontologies that are most similar to the work described below are EXACT [?] and the Semanticscience Integrated Ontology [?]. Both are motivated by a need to describe scientific protocols and experiments. Where they differ from what we are proposing here is that they describe *sets* of actions in scientific protocols and experiments, whereas we are proposing to represent *sequences* of actions, or steps in a procedure, if you like. Relations that describe orderings of actions (e.g., ‘precedes’ [?]) are not applicable to sequences since these relations are transitive.

The Molecular Methods Database (MolMeth) is a database which contains scientific protocol ontologies that conform to a set of laboratory protocol standards [?].

6.3 Procedure-oriented Ontology

We propose a framework for procedure-oriented ontologies that explicitly identify all steps of an experimental procedure and provide a set of relations to describe the relationships between the steps of an experimental procedure. The novelty of this approach is to allow creating a sequence of events (or steps in a procedure) using the ontological concept of "something occurs before". So, in order to accomplish that we need to have an ontological concept of "sequence". This is very significant concept because one cannot simply call a sequence of events "a sequence" unless these events happen step by step in some sort of ordering.

This approach will be used to provide the necessary information about the experimental procedures for Knowledge Base systems with the required knowledge about experimental processes. There are manuals of standard procedures in biochemistry [**?**, **?**] which in turn will help in building ontologies. See Fig. 6.3 which details the first steps of gel purification.

6.4 Relations

We first need to examine the types of features that an experimental procedure needs for its definition.

A procedure is a *sequence* of *steps*. These steps can be totally ordered or partialyl ordered. Total ordering needs a means to represent the concept that one event precedes another event and this relation needs to be transitive. Because a procedure is a sequence of steps, there needs to be a means to represent the relation that one step immediately follows another step and this relation needs to be intransitive. These relations have been defined for OWL and are available from `http://www.ontologydesignpatterns.org/cp/`

`owl/sequence.owl`. Partial ordering is accomplished simply by allowing more than one step to follow or to precede another step.

Finally, we would like to be able to represent a subsequence of steps and be able to represent the choice of a subsequence from one or more possible subsequences. This 'oneOf' relation would need to be crafted depending on how many choices are available. If two choices, this relation is simply equivalent to exclusive or otherwise it is simply a generalization of the exclusive or.

We have developed the concept of "procedure" based on these underlying relations.

6.5 Case Study

We have designed a procedure-oriented ontology for Alkaline Agarose Gel Electrophoresis [?] using the set of relations described in the previous section.

Fig. 6.1 shows the first steps that are involved in preparing the agarose solution. As one can see from Fig. 6.2, the second step is describing the preparation of DNA samples. The relation between step 1 and step 2 is "partially ordered". One can have these two steps performed in any order (e.g., step 1 then step 2 or vice versa). In addition, each one of these main steps consists of several steps (mini-steps or sub-steps). For example, in Fig. 6.1, step 1.1 "adding the appropriate amount of powdered agarose to a measured quantity of H2O" has two options either in: an Erlenmeyer flask 'exclusiveOR' a glass bottle. So we have a relation that conveys the choice of using one container or another. So, we will have two different sequences of steps: *If* "an Erlenmeyer flask" is selected *then* 'directlyFollows' "loosely plug the neck of the Erlenmeyer flask with Kimwipes"; *else if* "a glass bottle" is selected *then directlyFollows* "make sure that the cap is loose". As one can see, Fig. 6.2

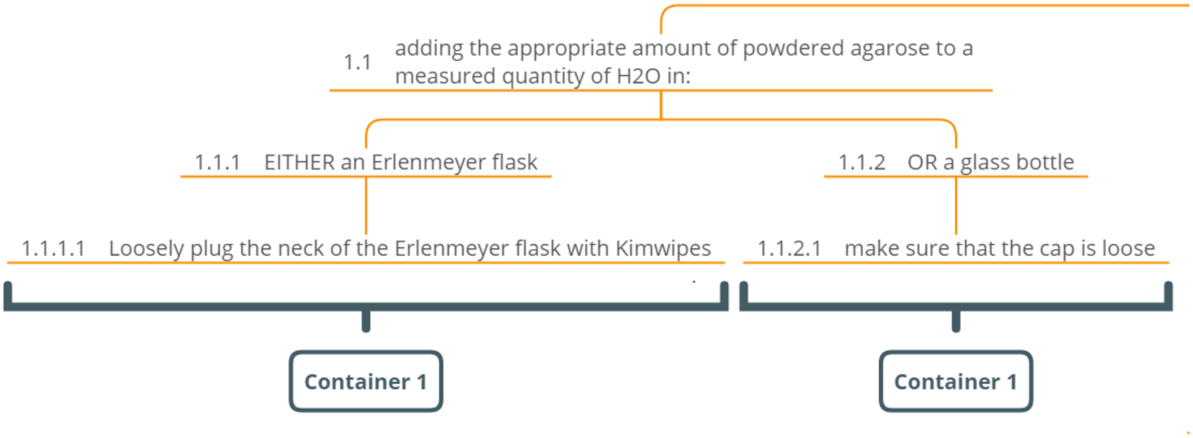
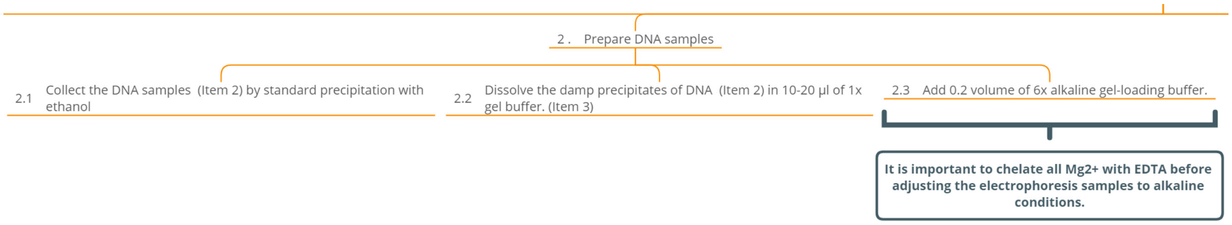


Figure 6.1: An example of alternative sub-sequences in steps for preparing Agarose solution. Note that in further steps of the procedure, Container1 will refer to either the flask or the bottle depending on which alternative has been taken.

shows a total ordered sequence.

We have proposed a procedure-oriented ontology that describes the relations and the sequence steps of experimental procedures in biochemistry. This will enrich the knowledge base systems with necessary information about experimental procedures that a scientist would automatically access such as instruments (e.g., buffers), materials (e.g., buffers). Most importantly, this approach is an important step toward our ultimate goal to analyze biochemistry articles.

Our interest in procedures has to do with understanding experimental procedures, but the ideas that are presented here could possibly be adapted to sequences of events in other systems, such as systems biology, because the intervention of a step could prevent a sequence of events from happening.



2 . Prepare DNA samples

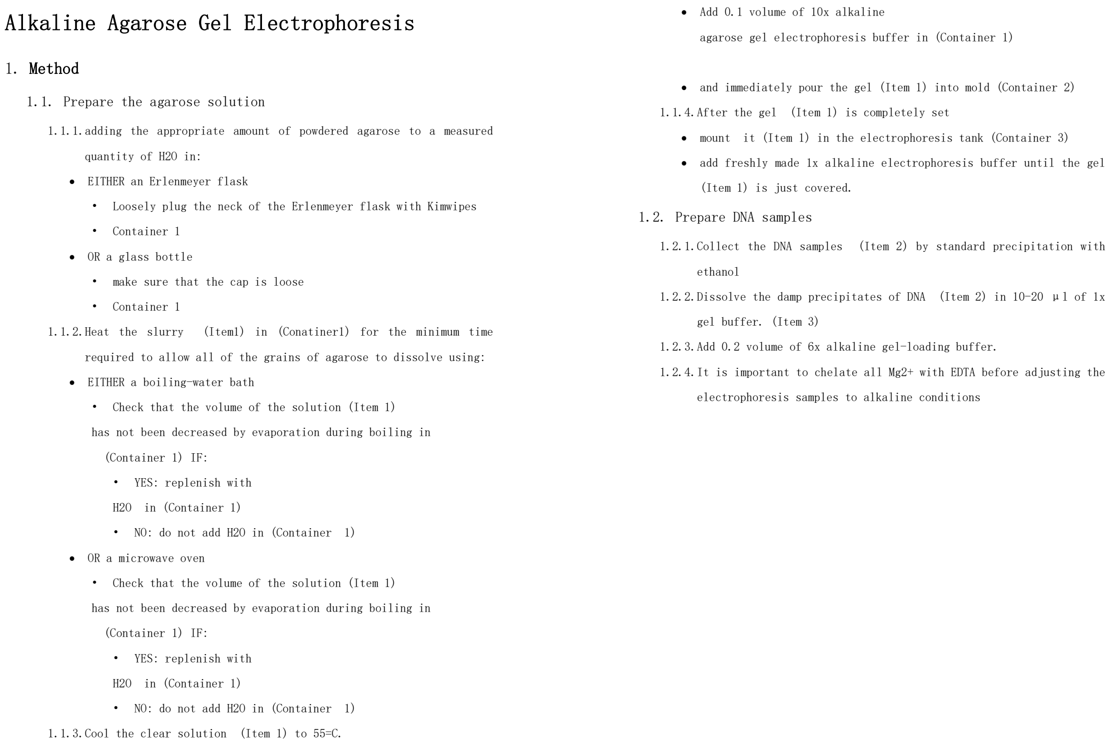
2.1 Collect the DNA samples (Item 2) by standard precipitation with ethanol

2.2 Dissolve the damp precipitates of DNA (Item 2) in 10-20 µl of 1x gel buffer. (Item 3)

2.3 Add 0.2 volume of 6x alkaline gel-loading buffer.

It is important to chelate all Mg2+ with EDTA before adjusting the electrophoresis samples to alkaline conditions.

Figure 6.2: Preparing the DNA samples which can be performed before or after the preparation of the Agarose solution shown in Fig. 6.1



Alkaline Agarose Gel Electrophoresis

1. **Method**
   1.1. Prepare the agarose solution
      1.1.1. adding the appropriate amount of powdered agarose to a measured quantity of H2O in:
      - EITHER an Erlenmeyer flask
        - Loosely plug the neck of the Erlenmeyer flask with Kimwipes
        - Container 1
      - OR a glass bottle
        - make sure that the cap is loose
        - Container 1

      1.1.2. Heat the slurry (Item1) in (Conatiner1) for the minimum time required to allow all of the grains of agarose to dissolve using:
      - EITHER a boiling-water bath
        - Check that the volume of the solution (Item 1) has not been decreased by evaporation during boiling in (Container 1) IF:
          - YES: replenish with H2O in (Container 1)
          - NO: do not add H2O in (Container 1)
      - OR a microwave oven
        - Check that the volume of the solution (Item 1) has not been decreased by evaporation during boiling in (Container 1) IF:
          - YES: replenish with H2O in (Container 1)
          - NO: do not add H2O in (Container 1)

      1.1.3. Cool the clear solution (Item 1) to 55=C.
      - Add 0.1 volume of 10x alkaline agarose gel electrophoresis buffer in (Container 1)
      - and immediately pour the gel (Item 1) into mold (Container 2)

      1.1.4. After the gel (Item 1) is completely set
      - mount it (Item 1) in the electrophoresis tank (Container 3)
      - add freshly made 1x alkaline electrophoresis buffer until the gel (Item 1) is just covered.

   1.2. Prepare DNA samples
      1.2.1. Collect the DNA samples (Item 2) by standard precipitation with ethanol
      1.2.2. Dissolve the damp precipitates of DNA (Item 2) in 10-20 μl of 1x gel buffer. (Item 3)
      1.2.3. Add 0.2 volume of 6x alkaline gel-loading buffer.
      1.2.4. It is important to chelate all Mg2+ with EDTA before adjusting the electrophoresis samples to alkaline conditions

Figure 6.3: The first steps of Alkaline Agarose Gel Electrophoresis

Chapter 7

Conclusion

we have develop a framework for automated argumentative-move detection consisting of two main components: (i) the definition of procedurally rhetorical verb-centric frame semantics and (ii) a formal computational representation of these frames. Such a framework provides a means for more in-depth automated analysis of the argumentative organization of this genre of texts than has previously been achieved. In our research, we have created annotated data sets and annotation guidelines for: (i) semantic roles, and (ii) argumentative moves. These annotated resources and guidelines are an important contribution to computational argumentation research.

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