

A Proposal for Chemical Information Retrieval Evaluation

Jianhan Zhu
University College London
Adastral Park Campus
Ipswich, IP5 3RE, UK
j.zhu@adastral.ucl.ac.uk

John Tait
Information Retrieval Facility
Vienna, Austria
john.tait@ir-facility.org

ABSTRACT

Based on the important progresses made in information retrieval (IR) in terms of theoretical models and evaluations, more and more attention has recently been paid to the research in domain specific IR, as evidenced by the organization of Geomatics and Legal tracks in TREC (Text REtrieval Conference). We think that now is the right time to carry out large scale evaluations on chemistry datasets in order to promote the research in chemical IR in general and chemical patent IR in particular. Accordingly, we propose the organization of a chemical IR track in TREC in order to address the challenges in chemical and patent IR. In this position paper, we present the research questions we will address in the proposed track, our initial plan of the proposed track, and the kind of search tasks we propose for the track. We focus on the design of a new chemical entity search consisting of two sub-tasks, i.e., chemical entity search and chemical entity relation search.

Categories and Subject Descriptors

H.3 [Information Storage and Retrieval]: H.3.1 Content analysis and indexing; H.3.3 Information Search and Retrieval; J.2 [Physical Sciences and Engineering]: Chemistry

General Terms

Experimentation, Measurement, Performance, Design

Keywords

Chemistry, chemical information retrieval, patent retrieval, prior art search

1. INTRODUCTION AND MOTIVATION

Domain specific information retrieval has increasingly become an important aspect of TREC as evidenced by the successful organization of the Geomatics Track from 2003 to 2007 [5], and the ongoing TREC Legal Track [1, 12]. Domain specific IR deserves special attention since specific domains have special characteristics and user information needs distinct from general purpose IR. In the light of these, we propose the organization of a chemical information retrieval track starting from 2009 addressing the many research questions in effective chemical information retrieval and extraction from large scale chemical datasets. The

datasets we want to look at consist of academic papers, chemical patent documents, and other related documents for example international standards.

Why now? In contrast to the significant efforts and advances made in general purpose IR research, much more remains to be done for chemical IR, and applying existing IR models and approaches to chemical IR. The same can be said of patent search at least in practice.

Witten [14] identifies the similarities between chemical IR and general purpose IR, as well as the distinct features in chemical IR. Along the same line, we will focus on studying the special features in chemical IR, and how to adapt techniques in general purpose IR to chemical IR.

Chemical IR can benefit from the existing research in general purpose IR, but we have identified the following distinct challenges that we will tackle in the proposed track.

Firstly, chemical names are often in different forms and one chemical can often be referred to in many different ways in text. Chemical name extraction and identification needs to be addressed in indexing and retrieval of chemical information. The ChemCS-seq project¹ is a successful step in this direction [11]. Besides, IR based on two-dimensional (2D) and three-dimensional (3D) structures of chemical molecules [7, 14] needs to be studied.

Secondly, chemical IR often deals with chemicals in terms of interactions and relations among chemicals, transformations of chemicals, and information about chemical properties. In these cases, chemical entity retrieval is preferred over document based retrieval. Natural language processing and domain knowledge based approaches has achieved some degree of success [8], however, chemical entity retrieval on large scale datasets still remains largely uninvestigated.

We observe a growing interest in extending document centric to entity centric retrieval. The TREC Expert Search Track has been investigating the evaluation of people retrieval since 2005 [3, 10], and INEX² (INitiative for the Evaluation of XML retrieval) 2007 initiated the XML Entity Ranking track for evaluating systems that summarize of entities [7]. A pilot entity relation search task in INEX 2008 will investigate how well systems can not only find entities relevant to a topic but also establish correct relations between them³. These efforts can complement our proposed track.

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¹ <http://chemcs-seq.net/>

² <http://www.inex.org/en.html>

³ <http://www.inex.org/en.html/tracks/entity-ranking/guidelines.asp>

Retrieval Of Medicinal Chemical Information

Minjie Lin



Retrieval Of Medicinal Chemical Information:

Whispering the Techniques of Language: An Emotional Journey through **Retrieval Of Medicinal Chemical Information**

In a digitally-driven earth wherever monitors reign great and instant connection drowns out the subtleties of language, the profound techniques and mental subtleties hidden within phrases usually get unheard. However, set within the pages of **Retrieval Of Medicinal Chemical Information** a interesting literary value blinking with natural emotions, lies an extraordinary quest waiting to be undertaken. Published by an experienced wordsmith, that wonderful opus attracts readers on an introspective journey, gently unraveling the veiled truths and profound impact resonating within the very material of every word. Within the emotional depths of the poignant evaluation, we can embark upon a genuine exploration of the book is primary subjects, dissect its captivating writing fashion, and fail to the strong resonance it evokes heavy within the recesses of readers hearts.

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