IntelliGenWiki: An Intelligent Semantic Wiki for Life Sciences

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Nov. 15th, Como, Italy

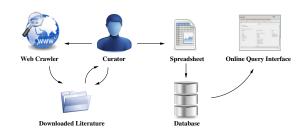
NETTAB 2012

Outline

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- 3 User Interface
- Application
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MOTIVATION: Curation of Biomedical Literature

- ▶ Finding and extracting relevant knowledge from the domain literature
- ▶ Manually refining and updating bioinformatics databases



MOTIVATION: Curation of Biomedical Literature

- ▶ Finding and extracting relevant knowledge from the domain literature
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- Manual literature curation is
 - Expensive → requires domain experts
 - ▶ Labour-intensive → ever growing amount of scientific publications
 - ▶ Error-prone → critical knowledge can be easily missed

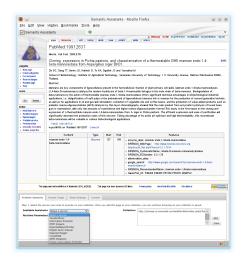




Enhanced Literature Curation Workflow Using IntelliGenWiki

- ▶ Text mining techniques integrated within the wiki environment
- ▶ Novel Human-Al collaboration patterns
- ▶ Producing semantic metadata
- ▶ Transform text into knowledge base

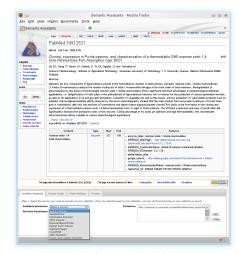
- Adopts the "Wiki" paradigm
 - Accessible via a web browser
 - Simple syntax (markup)
 - Open collaboration
- ▶ Based on the MediaWiki engine
 - Open source
 - Highly scalable
 - ▶ Extensible: Semantic MediaWiki



IntelliGenWiki User Interface



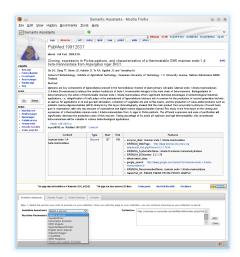
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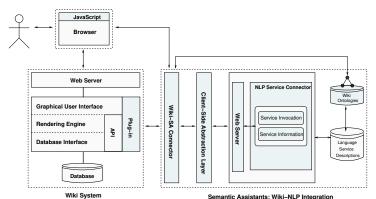
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- ▶ Open source software (AGPL3)





System Overview

- Front-end: Semantic MediaWiki
- Back-end: Wiki-NLP Integration [Sateli and Witte, 2012]
 - Comprehensive architecture based on the Semantic Assistants Framework [Witte and Gitzinger, 2008]
 - Seamless integration of various NLP capabilities within a wiki environment



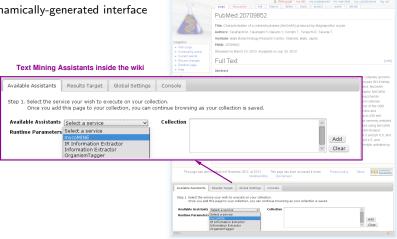
IntelliGenWiki Pages

▶ Each wiki page corresponds to a literature instance, e.g., abstract of a paper



The NIP Interface

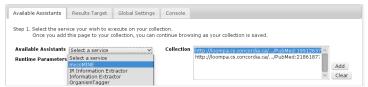
- ▶ The IntelliGenWiki NLP user interface offers various text mining services
- Customizing services at runtime
- Dynamically-generated interface



IntelliGenWiki NLP Services

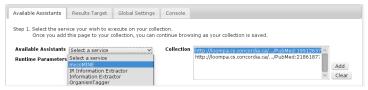
NLP Interface features

Multi-document Analysis



NLP Interface features

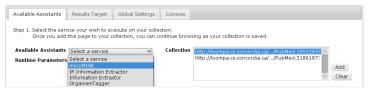
Multi-document Analysis



- ▶ Flexible handling of results
 - ▶ Writing to the same page as the resource
 - Writing to a different page in the wiki
 - ▶ Writing to an external wiki

NLP Interface features

Multi-document Analysis



- ▶ Flexible handling of results
 - ▶ Writing to the same page as the resource
 - Writing to a different page in the wiki
 - Writing to an external wiki
- Dynamic discovery of NLP services



Information Extraction

- Automatically extracting knowledge from text
- Various IE services
 - mycoMINE
 - OrganismTagger
 - Open Mutation Miner
- ► Enrichment of literature content with semantic markup

Example:

[[hasType::Enzyme|cellobiohydrolase]]

severely inhibited at pH 9.0. These results suggest that enhancement or inhibition of hydrolytic activities by cellobiose is dependent on the reaction mixture pH.

PMID: 20709852 Ø [PubMed - indexed for MEDLINE] PMCID: PMC2950481 Free PMC Article Ø mycoMINE on PMID: 20709852 Abstract (View) Ø

Content	Type	Start	End	Features
cellobiohydrolase	Enzyme	103	120	enzyma_aliax_calloliolytvfolase BRENDA_EsternalcName_silgoxyloglucan reducing_end_callobiohydrolase BRENDA_Echumber_3_z1,150 abbreviation_alion_silgoxyloglucan reducing_end_callobiohydrolase_com //asachtyrecallobiohydrolase_com //asachtyrecallobiohydrolase_com reducing_end_specific_callobiohydrolase_com //asachtyrecallobiohydrolase_com //asachtyrecallobiohydrol
Magnaporthe oryzae	Organism	143	161	NCB_Taxonomy_WebPage: http://www.ncbi.nlm.nih.gov/Taxonomy/Browser/www.ac.gi?nd=3188398.mode=info_d organism_scientific_name. Magnaporthe oryza organism_alias: Magnaponthe oryzae google_search: http://www.google.com //search?g=Magnaponthe+aryzae_G NCBI_Taxonomy_ID_318829

Semantic Entity Retrieval

- ▶ Unadorned wikis offer only keyword-based search
- ▶ What if we want to *discover* what's contained in the wiki?
 - ▶ e.g., "Which papers in this wiki mention an enzyme entity in their text?"

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- Solution: Querying the semantic metadata in the wiki
 - ▶ Search the wiki by semantic properties, e.g., entity type, generated by NLP services
 - Using special Semantic MediaWiki markup, called inline queries

```
{{#ask: [[hasType::Enzyme]]
| ?Enzyme = Enzyme Entities Found
| format = table
| headers = plain
| default = No pages found!
| mainlabel = Page Name
}}
```

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{{#ask: [[hasType::Enzyme]]
                                                  Property: Enzyme
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    Page Name

■ Enzyme Entities Found

    format = table
                                                   PMID: 20709852
                                                                                      Cellobiohydrolase
    headers = plain
                                                                                      Cellulases
     default = No pages found!
                                                                                      endoglucanases
    mainlabel = Page Name
                                                                                      β-glucosidases
                                                                                      Invitrogen
}}
                                                                                      DNA polymerase
```

Extrinsic Evaluation

User Study

▶ Is the integration of text mining assistants in a wiki environment actually effective?

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- ▶ User study within the Genozymes project context (www.fungalgenomics.ca)
 - ▶ Goal: Identifying and characterizing fungal enzymes
 - ▶ Dataset: 30 documents
 - ▶ Users: 2 expert biocurators
 - ▶ NLP Service: mycoMINE [Meurs et al, 2012]
 - ▶ Measure: Time spent on curation
 - Method: Comparison against time spent on manual curation

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Average Curation Time

Results:

Abstract Selection		Full Paper Curation		
no support	IntelliGenWiki	no support	IntelliGenWiki	
1 min.	0.3 min.	37.5 min.	30.6 min.	

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Conclusion: IntelliGenWiki was indeed efficient and reduced the paper selection and curation time by almost 70% and 20%, respectively.

What you can do now

- ▶ Install MediaWiki and Semantic MediaWiki extension
- Download and deploy the Wiki-NLP integration

What is next

- Cover other tasks, e.g.,
 - Quality assessment
 - ▶ Paper recommendation
 - Personalization
- Develop services for automatic import of literature, e.g., from PubMed
- □ Query the RDF in wiki from external applications



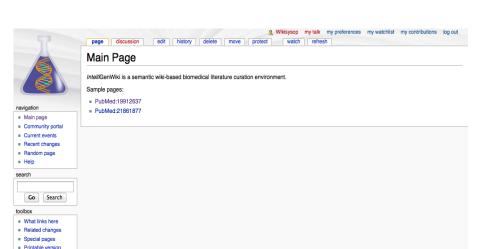
More Information

http://www.semanticsoftware.info/intelligenwiki

Acknowledgment

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- Caitlin Murphy and Sherry Wu, biocurators at the Centre for Structural and Functional Genomics (CSFG) at Concordia University, are acknowledged for their participation in the evaluation task.

Demo



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PubMed:19912637

Microb Cell Fact 2009:8:59

Cloning, expression in Pichia pastoris, and characterization of a thermostable GH5 mannan endo-1,4-beta-mannosidase from Aspergillus niger BK01.

Do BC, Dang TT, Berrin JG, Haltrich D, To KA, Sigoillot JC and Yamabhai M

School of Biotechnology, Institute of Agricultural Technology, Suranaree University of Technology, 111 University Avenue, Nakhon Ratchasima 30000,

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Mannans are key components of lignocellulose present in the hemicellulosic fraction of plant primary cell walls. Mannan endo-1,4-beta-mannosidases (1,4-beta-D-mannanases) catalyze the random hydrolysis of beta-1,4-mannosidic linkages in the main chain of beta-mannans. Biodegradation of beta-mannans by the action of thermostable mannan endo-1.4-beta-mannosidase offers significant technical advantages in biotechnological industrial applications, i.e. delignification of kraft pulps or the pretreatment of lignocellulosic biomass rich in mannan for the production of second generation biofuels, as well as for applications in oil and gas well stimulation, extraction of vegetable oils and coffee beans, and the production of value-added products such as prebiotic manno-oligosaccharides (MOS). A gene encoding mannan endo-1,4-beta-mannosidase or 1,4-beta-D-mannan mannanohydrolase (E.C. 3.2.1.78), commonly termed beta-mannanase, from Aspergillus niger BK01, which belongs to glycosyl hydrolase family 5 (GH5), was cloned and successfully expressed heterologously (up to 243 microg of active recombinant protein per mL) in Pichia pastoris. The enzyme was secreted by P. pastoris and could be collected from the culture supernatant. The purified enzyme appeared glycosylated as a single band on SDS-PAGE with a molecular mass of approximately 53 kDa. The recombinant beta-mannanase is highly thermostable with a half-life time of approximately 56 h at 70 degrees C and pH 4.0. The optimal temperature (10-min assay) and pH value for activity are 80 degrees C and pH 4.5. respectively. The enzyme is not only active towards structurally different mannans but also exhibits low activity towards birchwood xylan. Apparent Km values of the enzyme for koniac glucomannan (low viscosity), locust bean gum galactomannan, carob galactomannan (low viscosity), and 1.4-beta-D-mannan (from carob) are 0.6 mg mL-1, 2.0 mg mL-1, 2.2 mg mL-1 and 1.5 mg mL-1, respectively, while the kcat values for these substrates are 215 s-1, 330 s-1, 292 s-1 and 148 s-1, respectively. Judged from the specificity constants kcat/Km, glucomannan is the preferred substrate of the A, niger beta -mannanase. Analysis by thin layer chromatography showed that the main product from enzymatic hydrolysis of locust bean gum is mannobiose, with only low amounts of mannotriose and higher manno-oligosaccharides formed. This study is the first report on the cloning and expression of a thermostable mannan endo-1,4-beta-mannosidase from A. niger in Pichia pastoris. The efficient expression and ease of purification will significantly decrease the production costs of this enzyme. Taking advantage of its acidic pH optimum and high thermostability, this recombinant beta-mannanase will be valuable in various biotechnological applications.

PMID: 19912637 P

This page was last modified on 11 November 2012, at 06:46.

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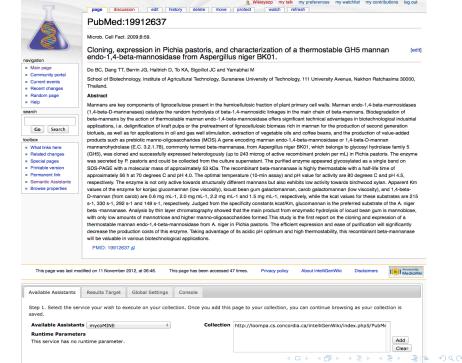
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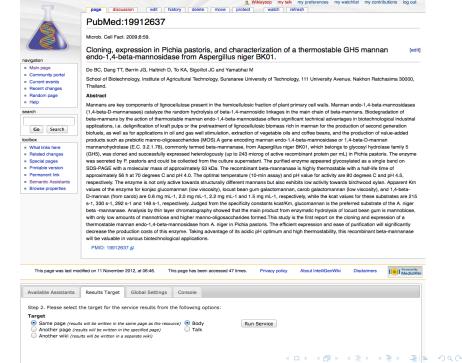
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PMID: 19912637 @

This page was last modified on 11 November 2012, at 06:46. This page has been accessed 47 times Privacy policy About IntelliGenWiki Disclaimers Powered By Martin/Wi Available Assistants Results Target Global Settings Console [Nov 13,2012 07:37] Console is ready! [Nov 13,2012 07:46] Number of documents to process: 1 [Nov 13,2012 07:46] Processing "http://loompa.cs.concordia.ca/intelliGenWiki/index.php5/PubMed:19912637" [Nov 13,2012 07:46] Bot successfully logged into the wiki. [Nov 13,2012 07:46] Retrieving page content... [Nov 13,2012 07:46] Invoking "mycoMINE" [Nov 13,2012 07:46] Service invocation finished. Writing the results... [Nov 13.2012 07:46] Results will be written in the body of the same page as the resource. [Nov 13,2012 07:46] Execution finished. 4 D > 4 B > 4 E > 4 B > 9 Q P



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mycoMINE on /PubMed:19912637 (View) re-

Content	Type	Start	End	Features
mannanases	EnzymeStats	588	598	Most_Frequent_BRENDA_EC_Number: 3.2.1.78 #_Distinct_Enzymes: 8 Most_Frequent_Enzyme: mannanase Most_Frequent_Enzyme_score: 6 #_Distinct_BRENDA_EC_Number: 3 #_Distinct_BRENDA_EC_Numbers: 3
mannan endo-1,4- beta-mannosidase	Enzyme	127	159	enzyme_alias: mannan endo-1.4-beta-mannosidase BERINDA_MOPage: http://www.bende-enzymes.org //phi/result_fist.php-?enco-4.2.1.78 @ BERINDA_SystematicName: 4-beta-0-mannan mannanohydrolase BIERINDA_ECNumber: 2.2.1.78 abbreviation_alias: groope_search: http://www.google.com/search?q-mannan+endo-1,4-beta-mannosidase BIERINDA_RecommendedName; mannan endo-1.4-beta-mannosidase BIERINDA_RecommendedName; mannan endo-1.4-beta-mannosidase SwassPreU_D_P49442 P49445 P51529 P5527 957527 G0MPU_Z

