# Semi-automatic Population of a Pharmaceutical Company Ontology



Master Thesis

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# Outline

- 1. Motivation
- 2. Contribution
- 3. System Overview
- 4. Triplet extraction
- 5.Conflicts
- 6.Evaluation
- 7. Patent Use Case
- 8. Further Work
- 9. Conclusion

# Motivation

- Competitive intelligence
  - Take informed decisions and to correctly evaluate risks, markets, opportunities, their and their competitors weaknesses and strengths
  - *Who* is my competitor?
  - The lack of a M&A ontology
- Ontology structure
- 'Googling' approach
  - 90% of the information needed for competitive intelligence could be found on the Internet (Teo and Choo, 2001)
  - "collective knowledge is much more powerful than individual knowledge" (Cimiano and Staab, 2004)

# Contribution

- Information acquisition from the WWW
- Company recognition (training)
- Pattern based relation recognition
- Company synonyms and preferred terms
- Filtering mistakes
- Consistent ontology building
- Evaluation





#### Overview

Innut Fields	Annotated Chinnets
	Annotated snippets
Search Company : Bristol Myers Squibb	ZymoGenetics was acquired by Bristol – Myers Squibb October 13 of last year for \$9.75 per
acquired_direct2 🔻 Search	share , and Isilon Corp. was purchased by EMC Corp. on December 21
left	Edit Ont entry
⊖ right	Mar 7, 2012 ZYMOGENETICS, INC (acquired by Bristol – Myers Squibb ) – . Atlanta, GA
Type a name and press Enter/Search.	Edit Ont entry
Edit Pane	Jan 11, 2012 and another significant ' pearl ', ZymoGenetics , was acquired . Fitch does
Marto 710, 10 201210, 10, 10, 7YMOCENETICS11, 11, INCL1 /10	recognize Bristol – Myers Squibb 's efforts since 2007 to strengthen the
acquired 3 by/3 Bristol 1 - 1 Myers 1 Squibb 1) 0 - 0 . 0 Atlanta 0	Edit Ont entry
,  0 GA 0 .  0 2007 9 to 0 2009 9 .  0 • 0 Exceeded 0 100 0 % 4	Mar 1, 2011 Previously, he was chief executive officer at ZymoGenetics Inc (acquired
sales 0 and 0 management 0 objectives 0 0 . 0	by BMS ), chief scientific officer at Seattle Genetics , and senior vice
	Edit Ont entry
	Jan 11, 2012, and another significant ' pearl ', ZymoGenetics , was acquired . Fitch does
	recognize Bristol – Myers Squibb 's efforts since 2007 to strengthen the
	Edit Ont entry
	Jul 19, 2011 In October 2010, ZymoGenetics was acquired by Bristol – Myers Squibb .
	Posted by Tracy Sferra , Course Coordinator • Email ThisBlogThis !
	BristolMyersSquibb acquired ZymogeneticsInc
Patroin Model Pafrach Add To Troin Cat Now	Add Rellation Add Company
Refresh Auu to train Set Now	







#### Overview

#### Novartis AG - Knowmore.org

knowmore.org/wiki/index.php?title=Novartis\_AG
8 Jul 2011 – The Company is based in Basel, Switzerland. In July 2008, Novartis AG
acquired a 25% stake in Alcon, Inc. from Nestle SA.

#### Novartis AG | Private Company Financial Research | PrivCo.com

www.privco.com/private-company/novartis-ag

PrivCo's M&A Activity table for Novartis AG displays the mergers and acquisitions involving Novartis AG, for example if **Novartis AG acquired** or was acquired by ...

#### Alcon - Advanced Vision Technologies of Golden, Colorado

www.avtlens.com/#!alcon

Novartis AG acquired its 77 percent majority ownership in a two step transaction with Nestlé S.A. In July 2008, Novartis purchased from Nestlé S.A. ...

#### "Switzerland's Novartis AG" Search - The Business Journals

www.bizjournals.com/search?q=%22Switzerland's+Novartis... When Switzerland's **Novartis AG acquired** Chiron Corp. in 2005, investors, city planners, and Chiron's then-2,300 local employees were wondering what would ...



#### Overview Annotated Snippets Input Fields Search Company : Bristol Myers Squibb ZymoGenetics was acquired by Bristol – Myers Squibb October 13 of last year for \$9.75 acquired\_direct2 Ŧ Search share, and Isilon Corp. was purchased by EMC Corp. on December 21 ... Edit Ont entry Ieft Mar 7 , 2012 ... ZYMOGENETICS , INC ( acquired by Bristol – Myers Squibb ) – . Atlanta , GA 🔘 right 2007 to 2009 . • Exceeded 100 % sales and management objectives ... Type a name and press Enter/Search. Edit Ont entry Edit Pane Jan 11, 2012... and another significant 'pearl', ZymoGenetics, was acquired. Fitch does recognize Bristol - Myers Squibb 's efforts since 2007 to strengthen the ... Mar[9 7]9, [9 2012]9...]0. [0 ZYMOGENETICS]1, [1 INC]1 ([0 ٠ acquired[3 by]3 Bristol[1 - [1 Myers]1 Squibb[1 )[0 - [0 .[0 Atlanta]0 Edit Ont entry [0 GAI0 .]0 2007[9 to]0 2009[9 .]0 •]0 Exceeded[0 100]0 %[4 Mar 1, 2011... Previously, he was chief executive officer at ZymoGenetics Inc (acquired sales[0 and[0 management[0 objectives[0 ...[0 ..[0 /BMS ) , chief scientific officer at Seattle Genetics , and senior vice ... Edit Ont entry Jan 11, 2012... and another significant 'pearl', ZymoGenetics, was acquired. Fitch does recognize Bristol - Myers Squibb 's efforts since 2007 to strengthen the ... Edit Ont entry Jul 19, 2011... In October 2010, ZymoGenetics was acquired by Bristol - Myers Squibb Rosted by Tracy Sferra , Course Coordinator • Email ThisBlogThis ! BristolMyersSquibb acquired ZymogeneticsInc Add Rellation Add Company Add To Train Set Now Retrain Model Refresh



#### Overview

Input Fields	Annotated Snippets
Search Company :     Bristol Myers Squibb       acquired_direct2        Search	ZymoGenetics was acquired by Bristol – Myers Squibb October 13 of last year for \$9.75 per share , and Isilon Corp. was purchased by EMC Corp. on December 21
<ul> <li>right</li> <li>Type a name and press Enter/Search.</li> </ul>	Mar 7, 2012 ZYMOGENETICS, INC (acquired by Bristol – Myers Squibb) – . Atlanta, GA . 2007 to 2009. • Exceeded 100% sales and management objectives Edit Ont entry
Edit Pane         Mar 9 7 9 , 9 2012 9 0 . 0 ZYMOGENETICS 1 , 1 INC 1 ( 0 acquired 3 by 3 Bristol 1 - 1 Myers 1 Squibb 1 ) 0 - 0 . 0 Atlanta 0 , 0 GA 0 . 0 2007 9 to 0 2009 9 . 0 • 0 Exceeded 0 100 0 % 4 sales 0 and 0 management 0 objectives 0 0 . 0         sales 0 and 0 management 0 objectives 0 0 . 0	Edit       Ont entry         Jan 11, 2012 and another significant ' pearl ', ZymoGenetics , was acquired . Fitch does recognize Bristol – Myers Squibb 's efforts since 2007 to strengthen the         Edit       Ont entry         Mar 1, 2011 Previously, he was chief executive officer at ZymoGenetics Inc ( acquired by BMS ), chief scientific officer at Seattle Genetics , and senior vice         Edit       Ont entry         Jan 11, 2012 and another significant ' pearl ', ZymoGenetics , was acquired . Fitch does recognize Bristol – Myers Squibb 's efforts since 2007 to strengthen the         Edit       Ont entry         Jan 11, 2012 and another significant ' pearl ', ZymoGenetics , was acquired . Fitch does recognize Bristol – Myers Squibb 's efforts since 2007 to strengthen the         Edit       Ont entry         Jul 19, 2011       In October 2010, ZymoGenetics was acquired by Bristol – Myers Squibb .         Posted by Tracy Sferra, Course Coordinator - Email ThisBlogThis !           Array           BristolMyersSquibb acquired ZymogeneticsInc
Retrain Model Refresh Add To Train Set Now	Add Rellation Add Company





#### Overview

Members list (inferred)	Annotations Usage	
Members list	Annotations: BristolMyersSquibbCompany	
Members list: BristolMyersS(UEDE	Annotations 🛨	▲
* *	synonym [language: en]	
ReneCareInternationalLic	Bristol – Myers . Squibb	
	s non m. Hanguage: anl	
BostonScientificCorpRus	Bristal Myors Squibb	
BostonScientificCorporati		
BoyleMedicalCorp	synonym [language: en]	
BovitrumAbAntiobesityD	Bristol – Myers Squibb Co	
BoxerAcquisitionInc	synonym [language: en]	
BrahmsDiagnosticaGmbh	Bristol – Myers Squibb Co.	
BrahmsDiagnosticaLlc	superior language: en]	000
BrahmsHoldingGmbh	Bristel Myors Squibb Company	
🔷 BrasilLtda	Bilstor - Myers squibb company	
🔷 BraskemSa	synonym [language: en]	
BraunMedicalInc	Bristol – Myers Squibb Company.	
BraunMelsungenAg	synonym [language: en]	
BravoHealthinc	Bristol – Myers Squibb.	
BreathLtd		000 -
BridgeMedicalInc	<u> </u>	
Bridgecolnc	Description: BristolMyersSquibbCompany 🔲 🗐 💷	Property assertions: BristolMyersSquibbCompany 🛛 🔳 💷 🗵
BristolLic		
BristolMeyersSquibbPhari	Company	
BristolMyersSquibbAb		BristolMversSquibbBelgiumSa
BristolMyersSquibbArgen     BristolMyersSquibbAustr		hasSubsidiary *Conclusions
BristolMyersSquibbRelai	Same Individual As	hasSubsidiary
BristolMyersSquibbBergit		BristolMyersSquibbPharmaceutica
BristolMyersSquibbbv	Different Individuals 🐨	IsLimited
BristolMyersSquibbCaribl		hasSubsidiary ? @ X O
BristolMyersSquibbComp		BristolMyersSquibbNzLimited
BristolMyersSquibbDeCol		■hasSubsidiary ? ② × ○
BristolMyersSquibbDeGu		Oncology I nerapeuticNetworkinc
BristolMyersSquibbDomi		
BristolMyersSquibbEcuad		ompany
BristolMyersSquibbEestiA		hasSubsidiary
BristolMyersSquibbFarma		BristolMyersSquibbHoldings2002
BristolMyersSquibbFarma		Limited
BristolMyersSquibbGmbh		hasSubsidiary ? @ 20
BristolMyersSquibbHoldii		BristolMyersSquibbHoldingGerma
BristolMyersSquibbHoldii		
BristolMyersSquibbHoldir		*RristolMversSquibbPolskaSn

**Figure:** Screenshot of our ontology opened with Protege 4.2

# **Triplet Extraction**

- Triplets are property assertions stored as 3-tuples
  - (subject, relation type, direct object)
- 3-step triplet extraction
  - Tag companies
  - Tag indicator words for relations
  - Match semantic patterns
- Company annotation
  - Conditional random fields (courtesy to Dr. Katrin Tomanek)
  - Trained on ~2000 snippets
  - 85% precision (5 folds cross validation)
  - Bristol-Myers Squibb has acquired Adnexus Therapeutics, developer of a new class of ... Bristol-Myers Squibb also acquired Medarex Inc., a biotech company and a ...

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# Triplet Extraction (2)

- Tag indicator words
  - Exact formulations are prior defined by hand
  - Search expressions are a subset of the indicator expressions
  - Bristol-Myers Squibb has acquired Adnexus Therapeutics, developer of a new class of ... Bristol-Myers Squibb also acquired Medarex Inc., a biotech company and a ...
- Match semantic patterns
  - Inspired by *Hearst, 1992*
  - company (*otherTerms*){0, 5} indW (*otherTerms*){0, 5} company
  - Check the other terms
  - (BristolMyersSquibb, acquired, AdnexusTherapeutics), (BristolMyersSquibb, acquired, MedarexInc)

# Triplet extraction (3)

- Whole snippets (like in the previous example)
- Contextually decomposed snippets
  - "Merial, the Animal Health division of Sanofi, has acquired NewportLaboratories, a privately held company based in Worthington, Minnesota."
  - Context 0: Merial has acquired NewportLaboratories.
  - Context 1: Merial the Animal Health division of Sanofi
  - Context 2: Worthington, Minnesota
  - Context 3: NewportLaboratories, a privately held company based in Worthington
  - Courtesy to Elmar Hausmann

# Ontology building

- Structure
  - 1 Class
  - 4 relation types acquired, hasSubsidiary, hasMergerPart, holdsSharesBy
- Main problems
  - Identity matching (Novartis = Novartis AG)
  - Injectivity violations, cycles, incorrect/incomplete information
  - Entity tagging problems

# Identity matching

- Identification and merging of different name variations which refer to the same individual e.g. (AbbottLaboratories, acquired, KosPharmaceuticalCo); (AbbottLabs, acquired, TapPharmaceuticals)
- Assign synonyms & preferred terms
  - NovartisPharmaceuticalsCorporation: NovartisPharma, NovartisPharmaceuticals; NovartisAg: Novartis
  - Group names by root, get suffixes, assign preferred & synonyms
  - Based on the number of hits
  - Restriction: preferred terms always have a company suffix

### **Other Issues**

- Named entity filtering
- Triplet filtering
  - $treeSize\_parent | treeSize\_child < \delta$
  - hits\_parent / hits\_child < α</li>
  - (JohnsonSonInc, acquired, BayerAg) and h\_JohnsonSonInc = 35,600, h\_BayerAg = 2,790,000; st\_JohnsonSonInc = 1 and st\_BayerAg = 40
- Check for cycles
- Solve potential injectivity violations
  - Choose the most specific triplet (deepest leaf)
  - Prioritize companies with suffix
  - Occurence number of the triplets
    - occNo(triplet\_i) / occNo(triplet\_j) > 5



### **Evaluation Measures**

- Standard precision, recall, F1 score
- The **triplet-wise recall** is a self made measure
  - important that a triplet is retrieved, but not that it is retrieved from every single snippet in which it occurs
  - Apr 1 , 2009 ... Sanofi acquires Brazilian generics firm Medley for 500mm on Strategic Transactions , Apr-01-2009 . (snippet 1)
    - (Sanofi, acquired, Medley)
  - Dec 21 , 2009 ... Sanofi has acquired generic drug makers HelvepharmAg of Switzerland, MedleySa of Brazil and LaboratoriosKendrickSa of Mexico,... (snippet 2)
    - (Sanofi, acquired, HelvepharmAg)
  - *T-w recall* = **2/3**
  - Standard recall = 2/4

# **Evaluation: Triplet extraction**

We used 500 hand annotated snippets as gold standard.

	all	acquired	hasSubsidiary
Precision	84.97 %	82.93 %	87.21 %
Recall	58.10 %	61.26 %	59.06 %
F1 score	69.01 %	70.47 %	70.42%
Triplet-wise recall	86.21 %		

**Table1** : Evaluation of our triplet extraction with contextual sentence decomposition of the snippets.

	all	acquired	hasSubsidiary
Precision	82.52 %	85.39 %	82.86 %
Recall	67.46 %	69.09 %	70.16 %
F1 score	74.23 %	76.38 %	75.98 %
Triplet-wise recall	92.96 %		

Table2 : Evaluation of our triplet extraction an whole snippets.

#### Co-occurence

- The **simple co-occurence** takes all pairs of entities in a snippet as positives.
  - (NovartisAG, AlconInc), unordered
- The **typed co-occurence** also takes into account the difficulty of relation type disambiguation and subject/object identification.
  - (NovartisAG, holdsSharesBy, AlconInc), (NovartisAG, acquired, AlconInc), (NovartisAG, hasSubsidiary, AlconInc), (AlconInc, holdsSharesBy, NovartisAG), (AlconInc, acquired, NovartisAG), (AlconInc, hasSubsidiary, NovartisAG)
- Lower limit for precision and a upper limit for recall

Measure	Simple co-occurence	Typed co-occurence
Recall	80.55 %	80.55 %
Precision	31.96 %	5.56 %
F1 score	45.77 %	10.40 %

**Table3** : Co-occurrence results on whole snippets

# Ontology evaluation

Evaluated relations	Correct	Irrelevant	False
all	77.83 %	12.97 %	9.19 %
hasSubsidiary	93.9 %	3.66 %	2.44 %

**Table4** : Ontology evaluation on 300 "child" companies owned by 4 parent companies

- Correct: Acquisitions, subsidiaries or divisions which could be found on official web sites
- Irelevant: entity tagger problems e.g. *AtPhadiaUsInc, DoeIngallsIncMore* or incomplete names
- False: No relevant evidence could be found

Costs:

- On average ~2 queries per ontology entry
- Worst case scenario would be 8 queries per entry (2 test queries and 4 normalization queries)
- 5\$ for 125 triplets

#### Patent Use Case

- Broccoli is a semantic search engine which combines full text search and ontology search
- Developed by Prof. Bast's group
- 1.5 Mio European patent documents from MAREC database
- Simple entity recognition, contextual decomposition
- Our company ontology and YAGO ontology

Example of possible query formulations:

- What patents are assigned to Company X and subsidiaries?
- On which proteins does Company X work?
- Which patents about protein inhibition are held by private persons? (instead of companies)

#### Patent Use Case (2)



http://filicudi.informatik.uni-freiburg.de:6222/BroccoliPatents/

Which regulation methods patented Company X?

### **Further Work**

- Use a statistical model to evaluate the "trustworthiness" of a snippet (URL, writing style)
- Use a model to assign probabilities to already extracted triplets ("trustworthiness" of the snippet, occurrence number, hits number)
- Use more relations
- Solve temporal issues (i.e. reacquisitions)
- Completely automatize the process

# Conclusion

- 92.9% triplet wise recall shows that the information in snippets is accessible to extraction tools despite their structure and poor grammar
- given the (overall) unreliable nature of the information on the Internet, filtering techniques are needed
- < 10 % false relations in our ontology shows that even simple tests and conflict solving approaches such as ours can be efficient

### Thank you!

For your advices, time and attention.