Data Mining tools for Biomedical Discovery: a framework application in a Biotech Pharma Industry.

A case report of a working group

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Data Mining – Introduction and Aims

In the era of *big data*, Text Mining (TM) represents an essential tool to automate the process of the information retrieval, extraction, interpretation and analysis.

This study provides a practical example of using the TM tool in drug discovery and hypothesis generation.

We compared **Knime** and **R**, two web based open source and free tools, as useful methods in improving the workflow of information search in the Rheumatology field.

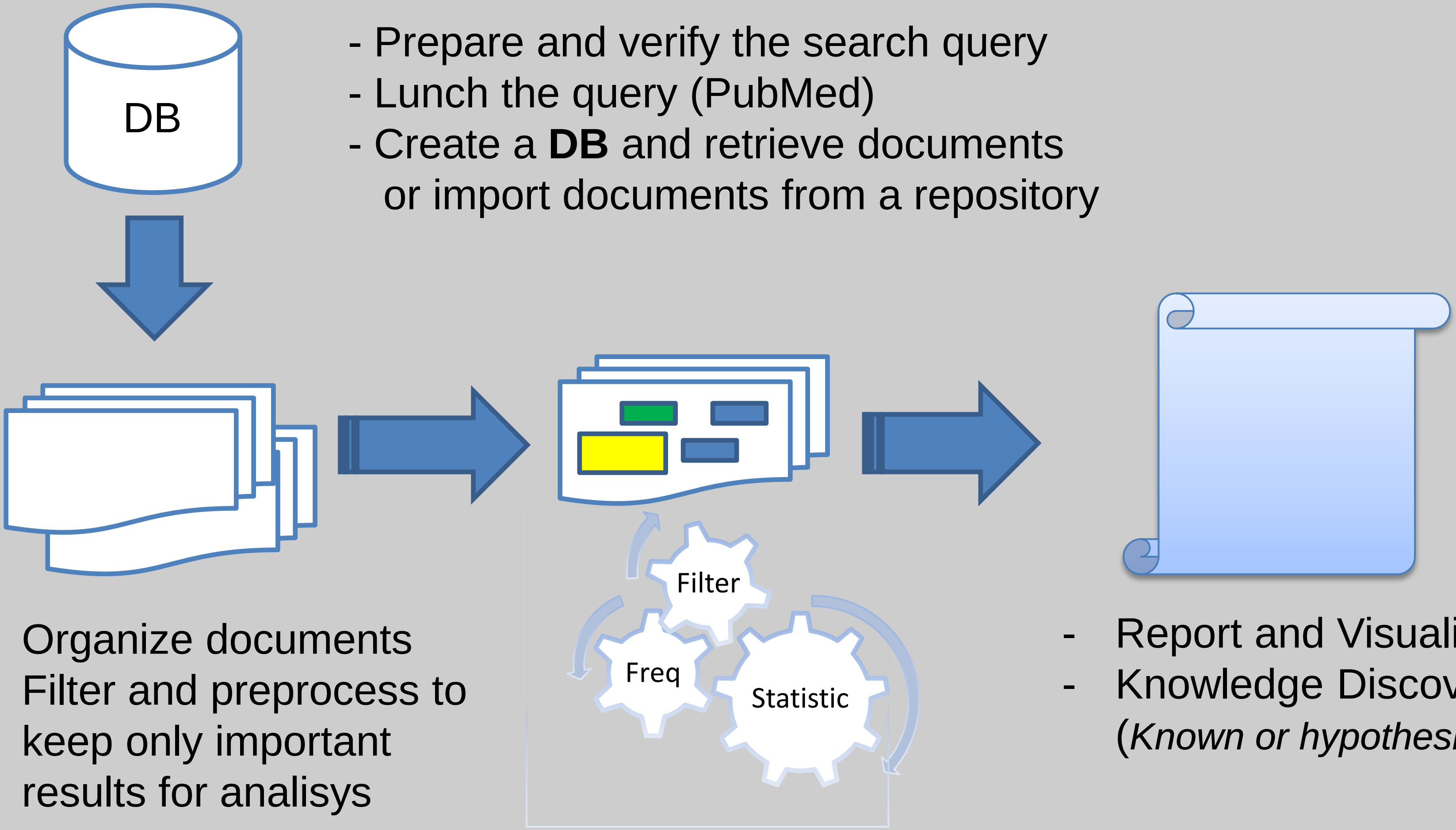
Data Mining - Query

We performed the following search query:

Osteoarthritis, Knee [MeSH*] AND *Humans* [MeSH] AND *Pain

in both systems, to search for new valuable target(s) in Knee OA.

General Text Mining Plan and Workflow



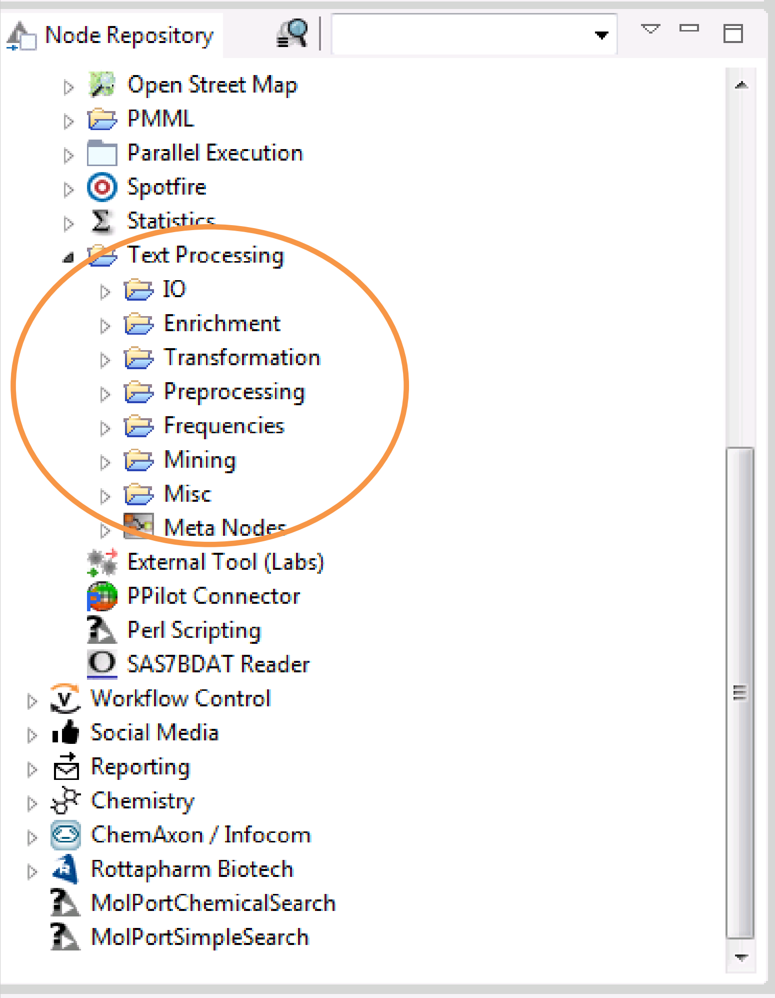
- Prepare and verify the search query
- Lunch the query (PubMed)
- Create a **DB** and retrieve documents or import documents from a repository

- Organize documents
- Filter and preprocess to keep only important results for analisys

- Tag terms(Abner), filter,
- analize for occurence and classify documents or extract relevant terms

- Report and Visualization
- Knowledge Discovery (*Known or hypothesis*)

Knime plugin

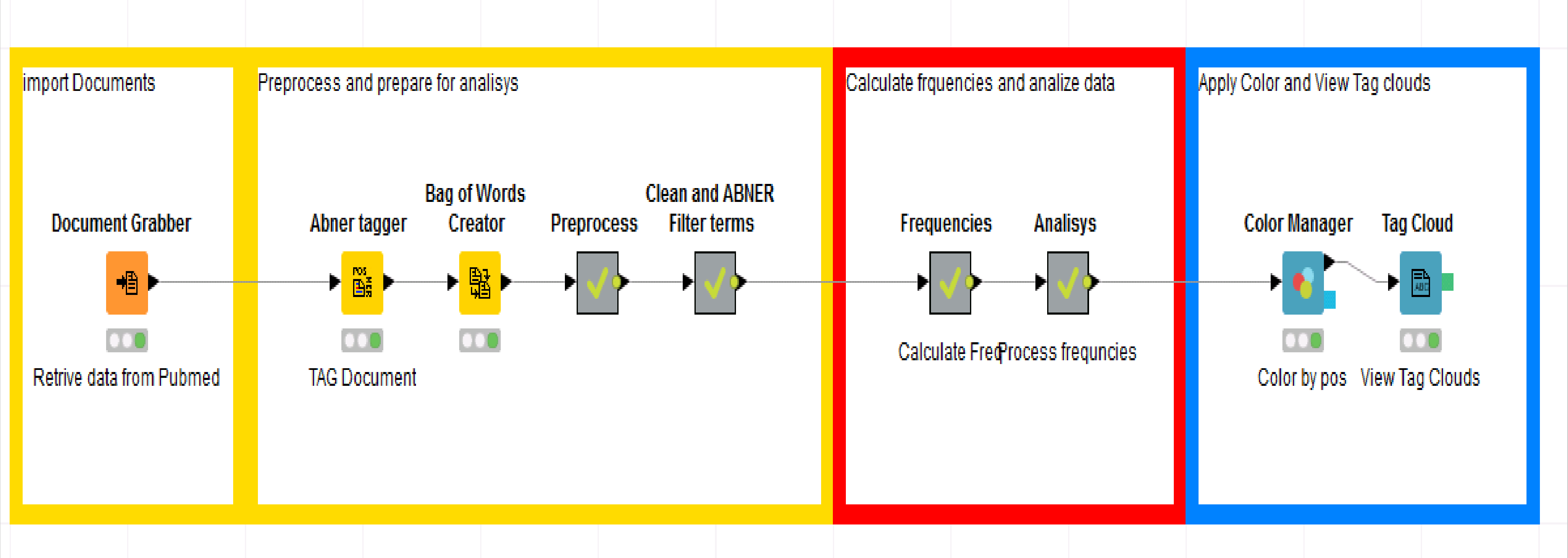


Node Repository

- Open Street Map
- PMML
- Parallel Execution
- Spotfire
- Statistics
- Text Processing
  - IO
  - Enrichment
  - Transformation
  - Preprocessing
  - Frequencies
  - Mining
  - Misc
  - Meta Nodes
- External Tool (Labs)
- PPilot Connector
- Perl Scripting
- SAS7BDAT Reader
- Workflow Control
- Social Media
- Reporting
- Chemistry
- ChemAxon / Infocom
- Rottapharm Biotech
- MolPortChemicalSearch
- MolPortSimpleSearch

- **IO** = Several Nodes are available for Query/Read documents
- **Enrichment** = assign Tags
- **Preprocess** = clean the «bag of words»
- **Frequencies** = Statistic analysis of frequency or co-occurence of Terms
- **Mining** = extract important terms to report

Case 1: Knime Abner tagger node



import Documents

Preprocess and prepare for analisys

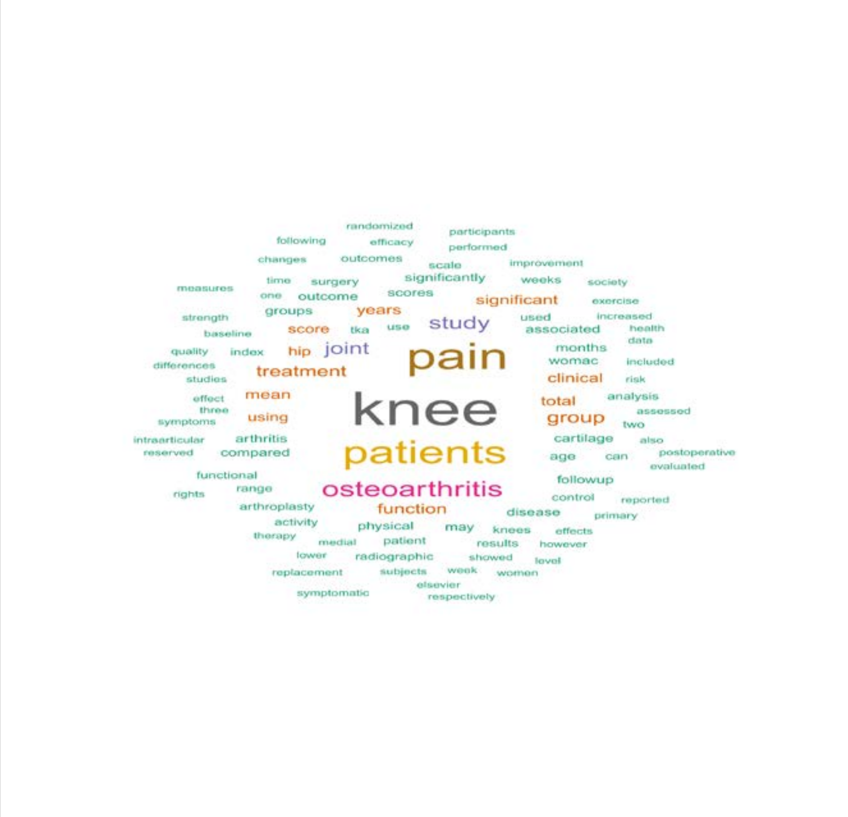
Calculate frquencies and analize data

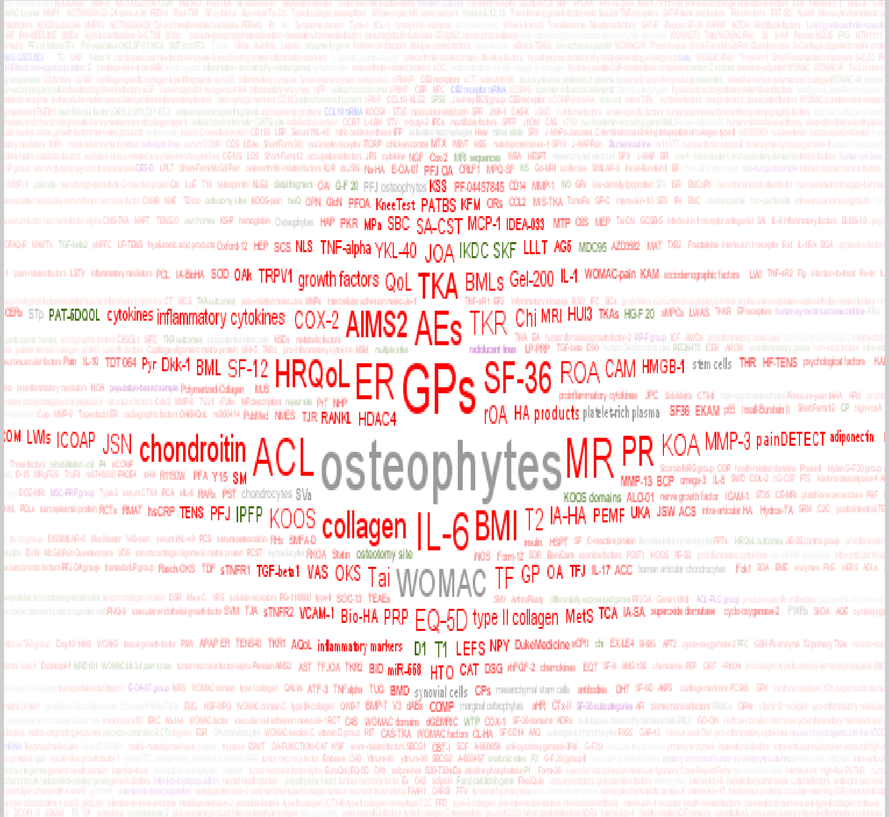
Apply Color and View Tag clouds

Case 1: Word Cloud Visualization

R: Word-cloud visualization

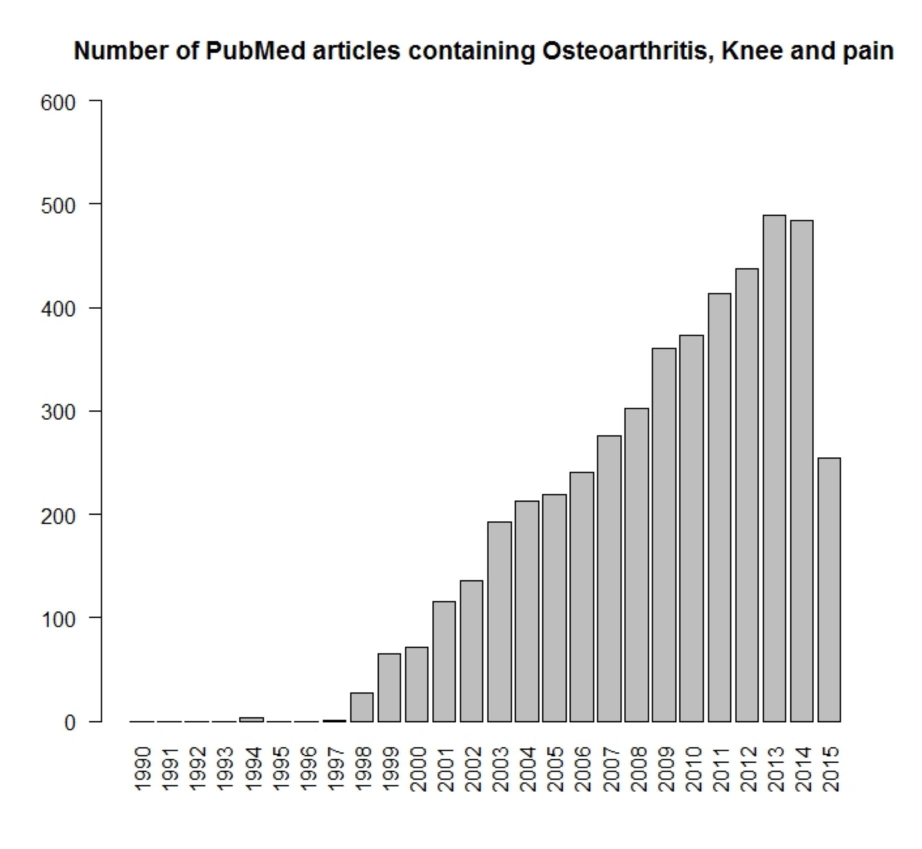
Knime: Word-cloud visualization (abner tagger)



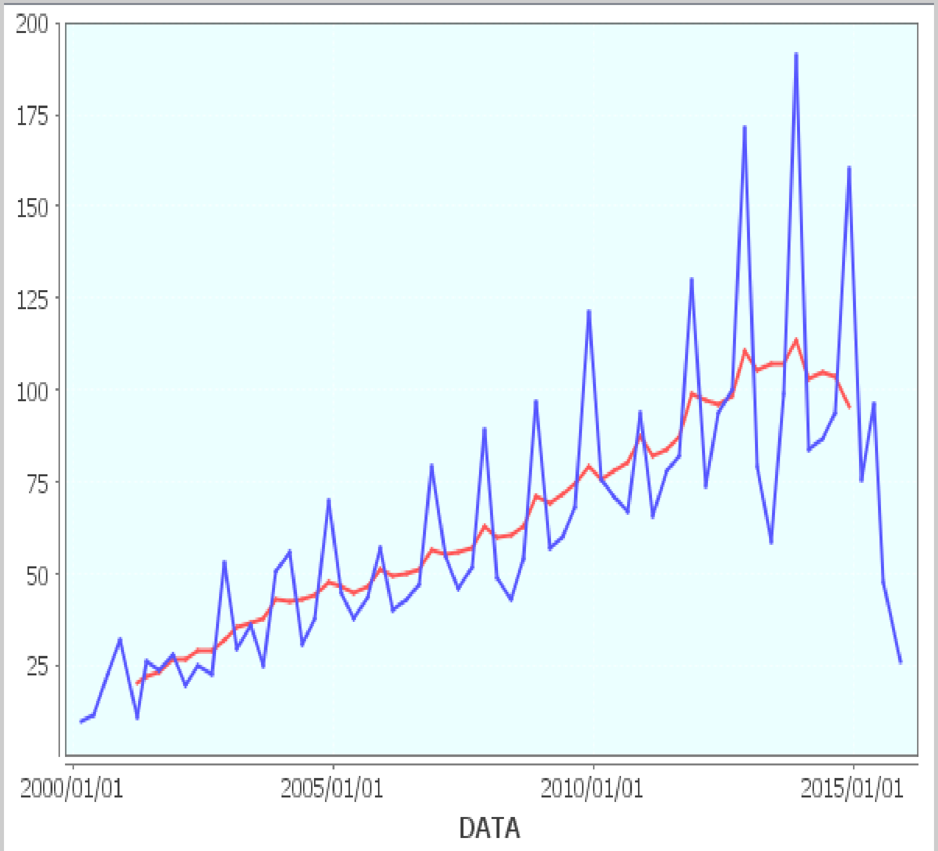


Case 2(a): temporal tendency in query

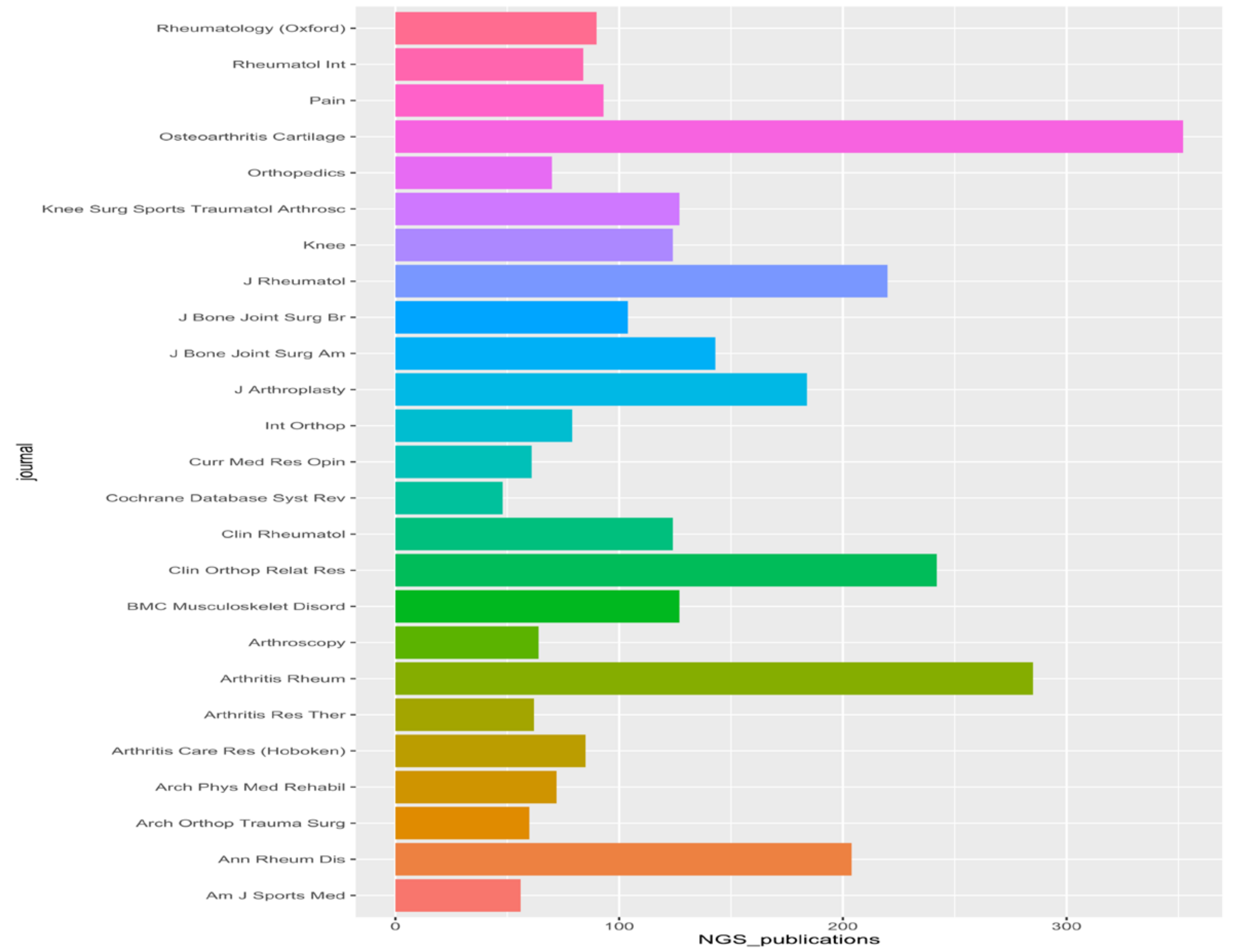
R:



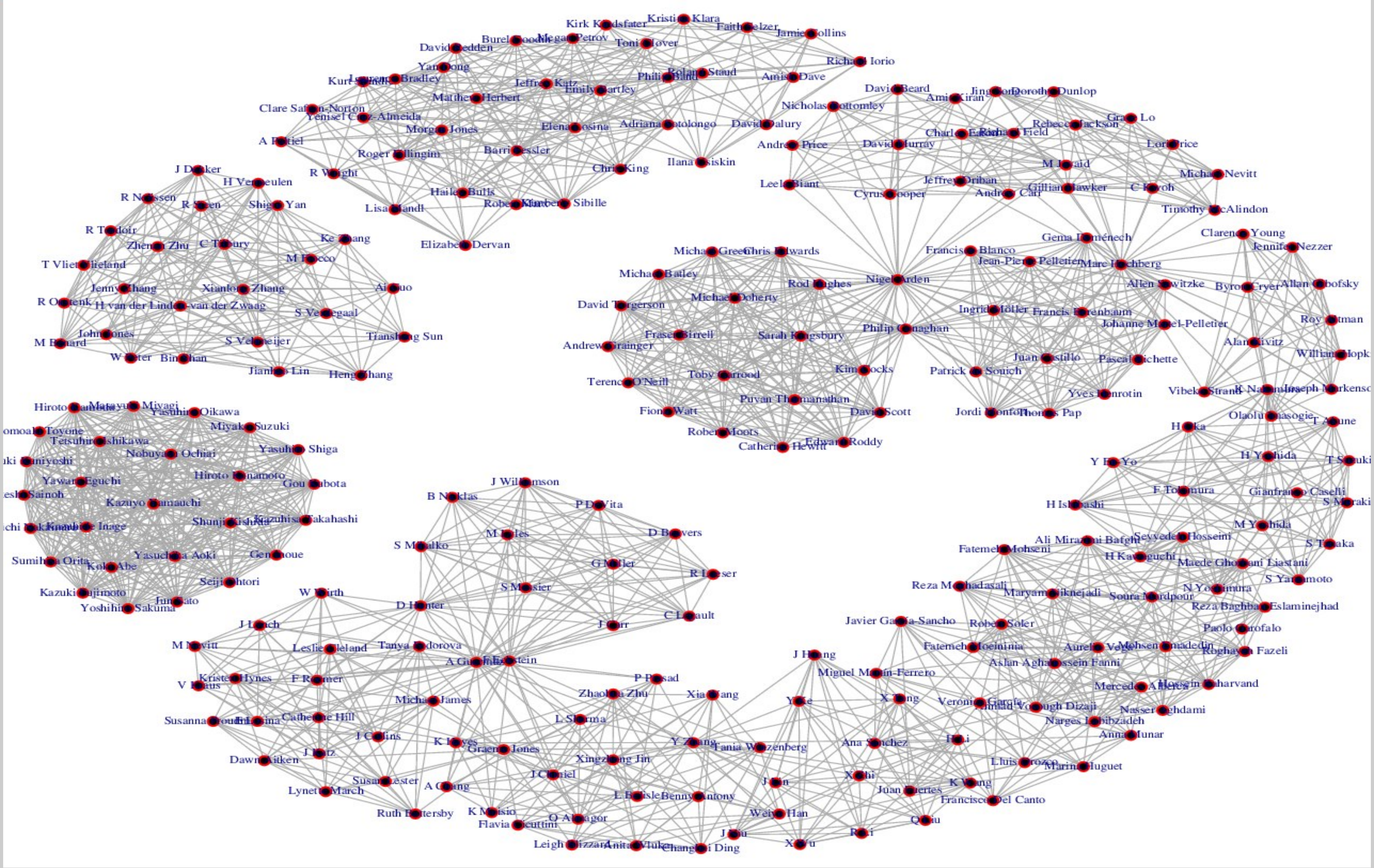
Knime



Case 2(a1): R - number of publications per journal

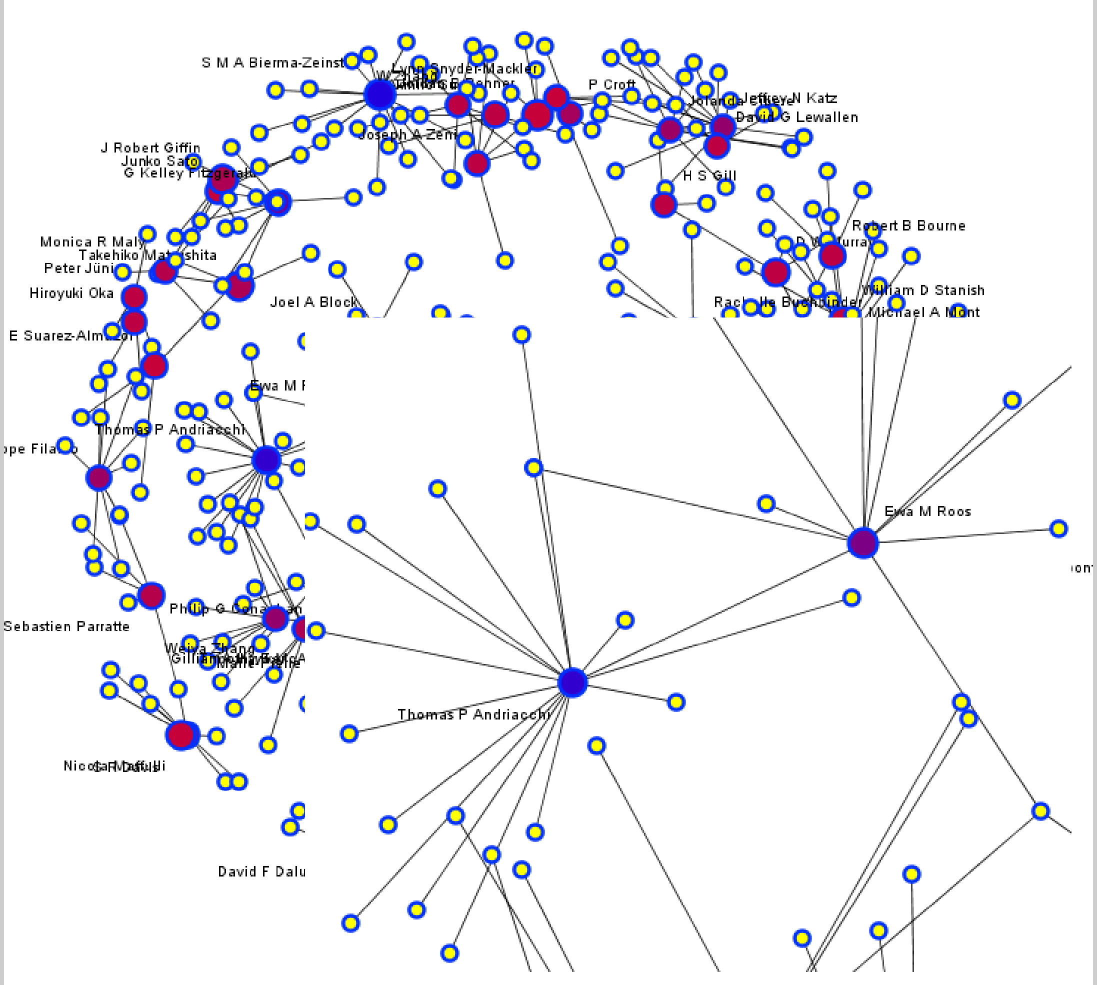


Case 2(b): R - Author network



Case 2(b): Author network

Authors' network related to No. of papers on Knee OA



Legend Color

● = High n° publications

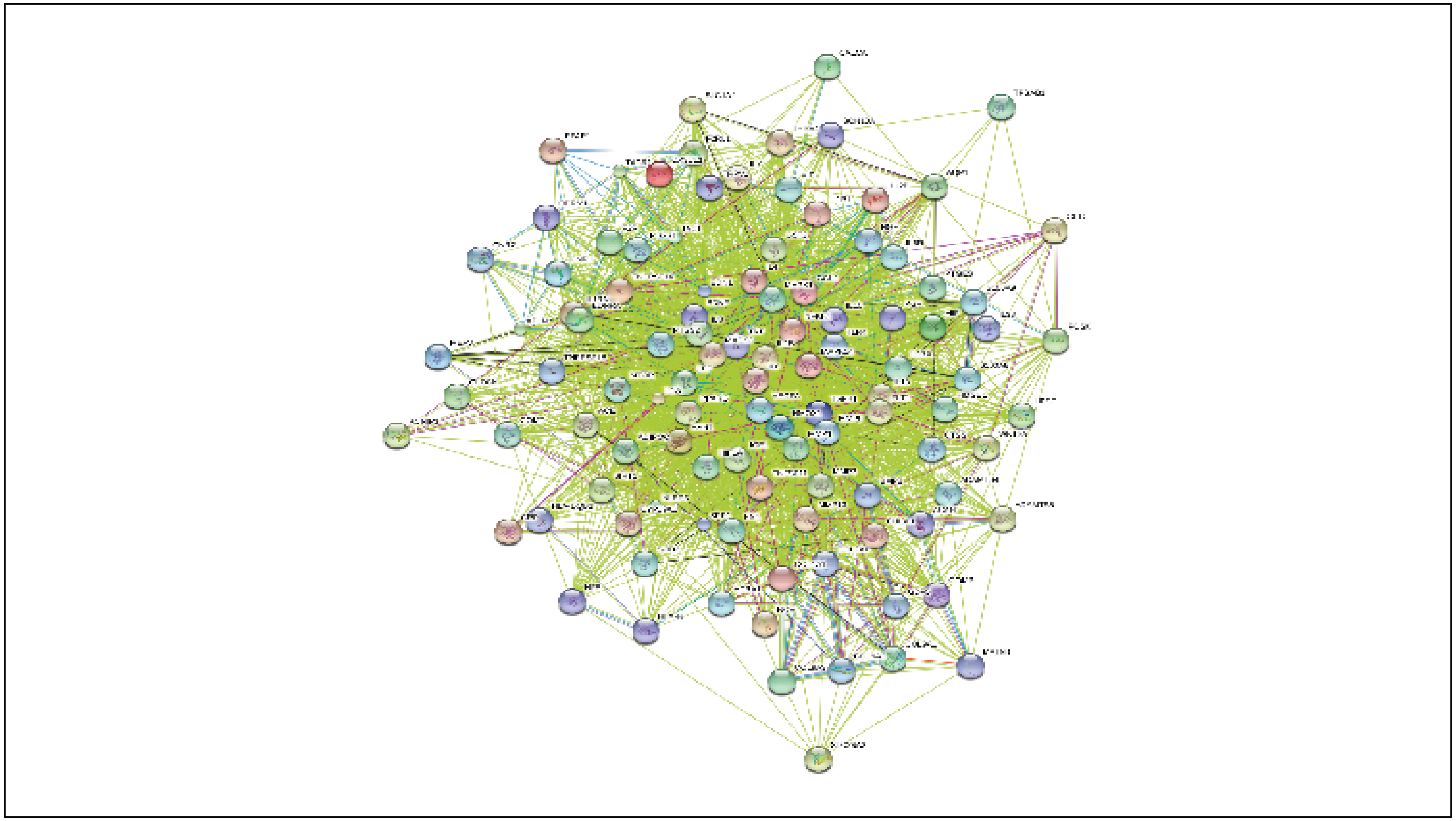
● = Medium n° publications

Case 4:
target discovery PP-interaction network

- Workflow can extract Protein-gene and Protein-Protein Interaction from literature.
- based on a custom dictionary of terms of interaction.
  - It is important to find out and extract the right Interactions
- The most «interesting» protein lists are sent to iHOP to investigate and compare the results

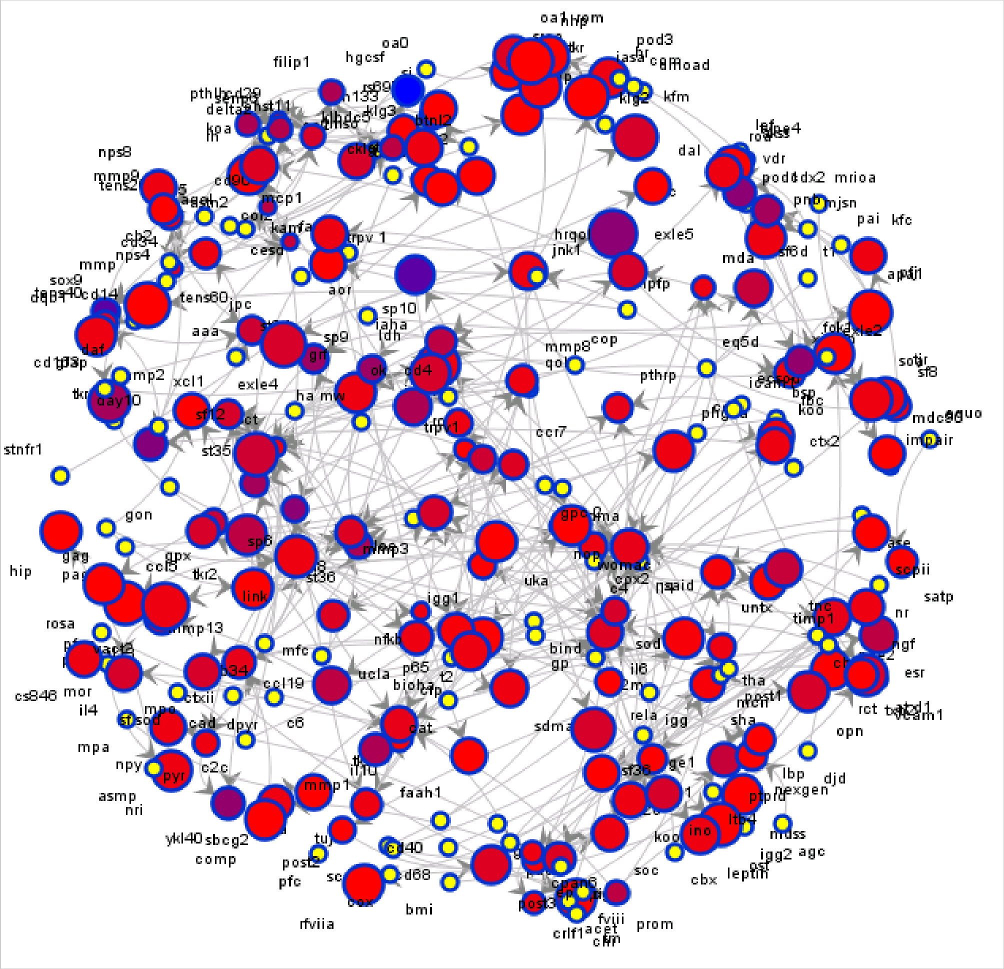
Case 4: target discovery PP-Interaction network by R

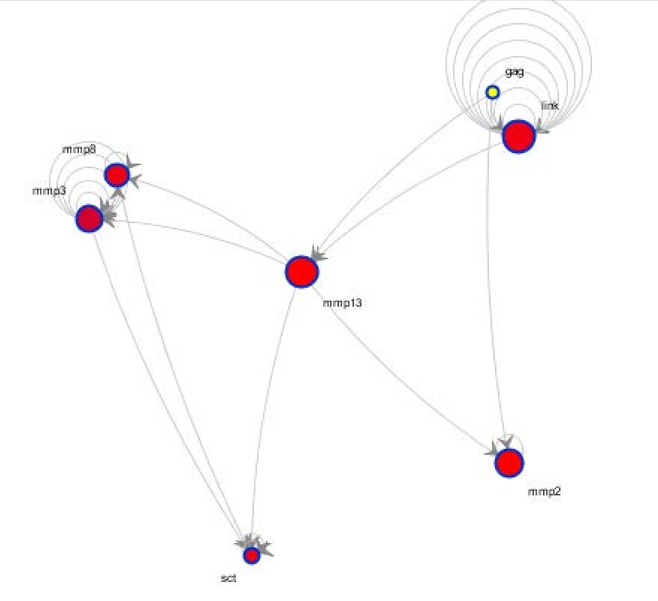
proteins: 200
interactions: 2492
expected interactions: 1021 (p−value: 0)



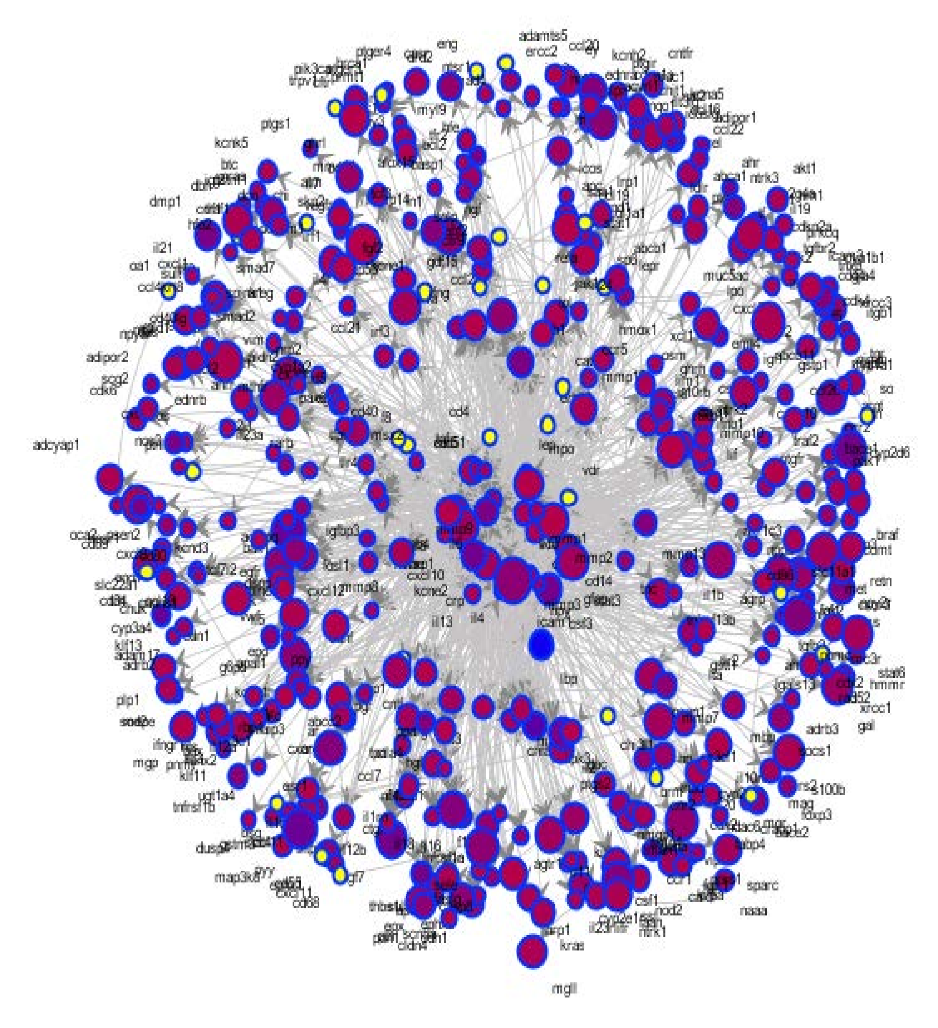
http://string−db.org/10/p/8344194184

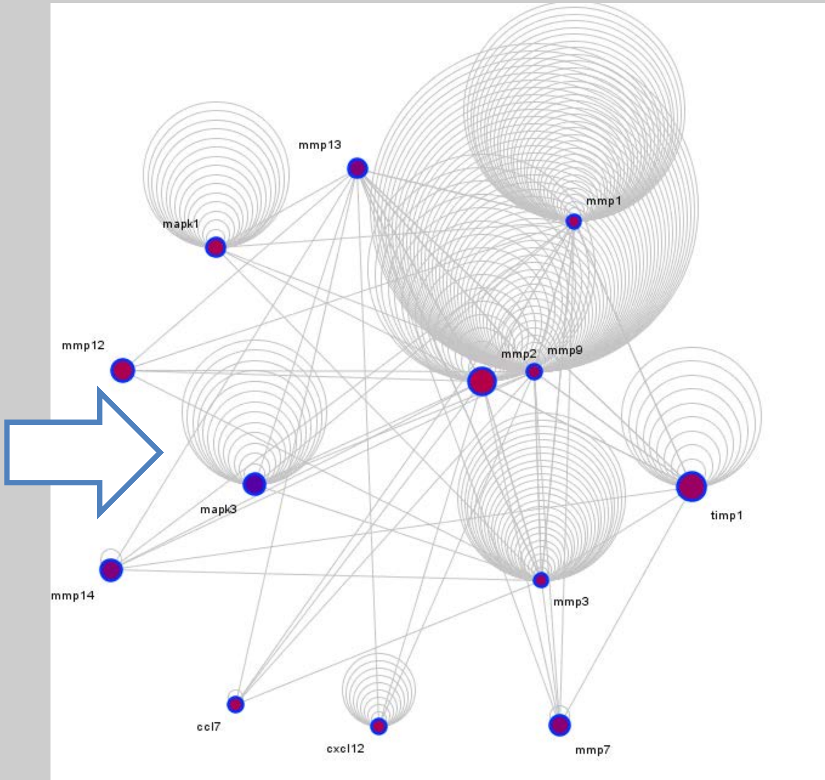
Case 4:
target discovery PP-Interaction network (knime)





Case 4:
target discovery PP-Interaction network (iHOP)





Conclusions

- TM brings knowledge from literature to identify known and new relationship between genes, pathways, drugs and diseases.
- TM is integration of different sources even in human ware
- A collaborative team with Biologists, Chemists, Statisticians, Librarians and Computer Technicians will be a new challenge in drug discovery.
- Biomedical Librarians can play a critical role in TM process, providing researchers access to taxonomy and vocabulary use or creation, and sharing content platform.

Rottapharm Biotech TM Team

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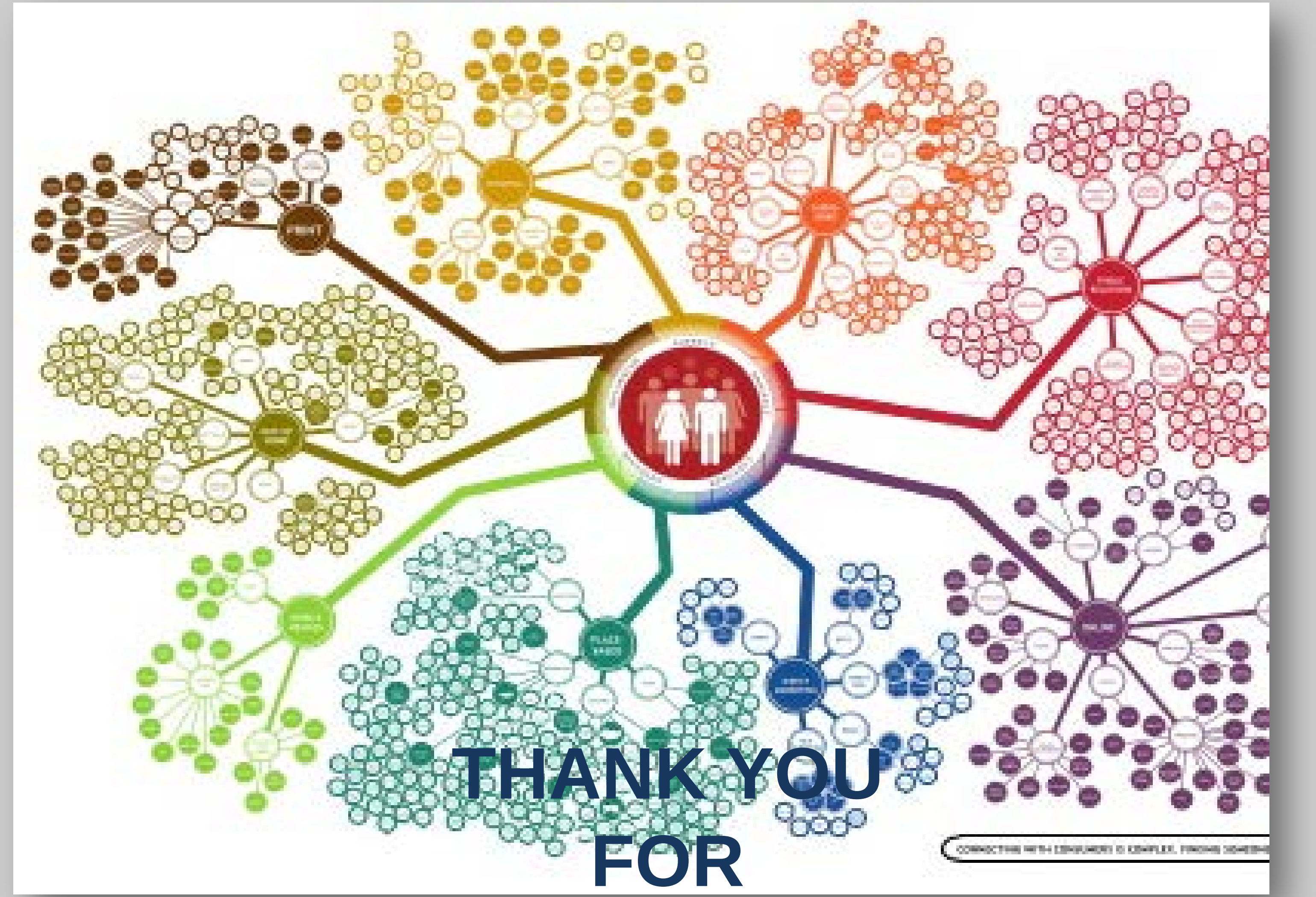
Francesca Gualtieri, Biomedical Librarian

Lucio Rovati, Medical Doctor

We would like to thank Fabrizio Arosio, computer Technician, for his helpful work.



THANK YOU FOR YOUR ATTENTION

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