



From the ELN to Data Warehouse

Applied to chemical reactions

Mercredi 12 Février 2014

Frank Hoonakker

- > **50 000** companies
- > **2 000** universities
- **600 000** chemists
 - 5,4 Billion € (consumables)
 - 300 reactions / chemist / years :

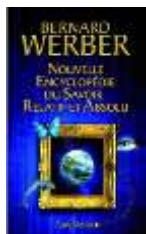
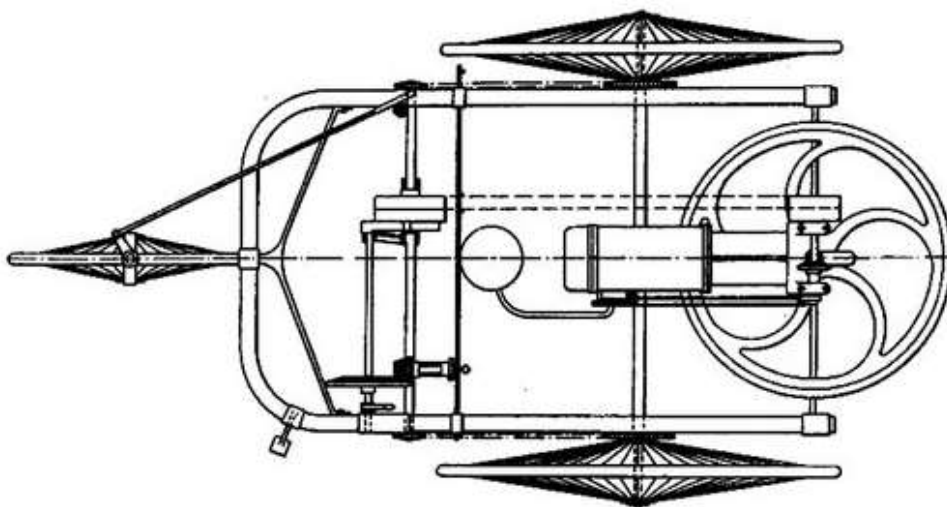
180 000 000 reactions / year

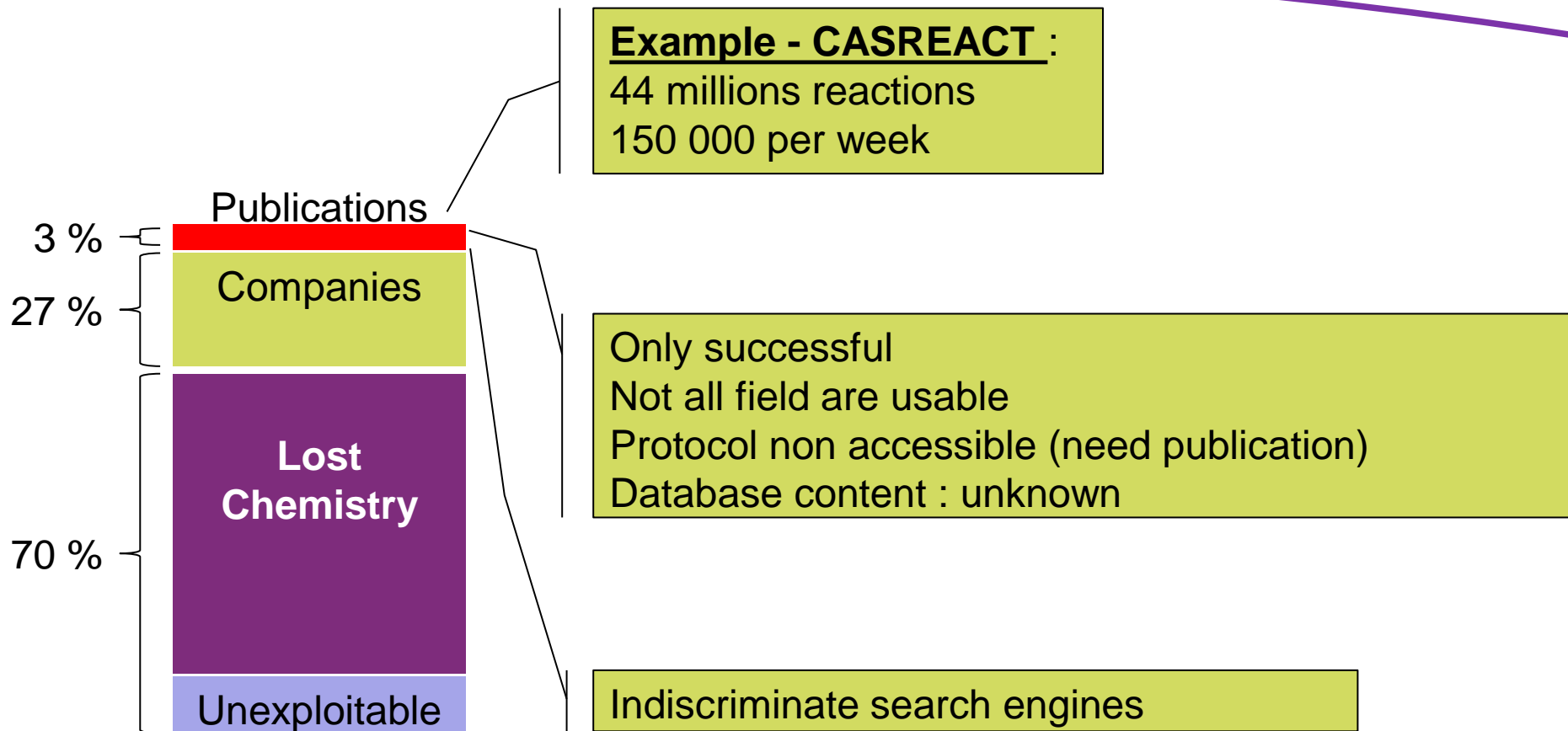
50% > failed reactions > 70%
~ 3% pulished

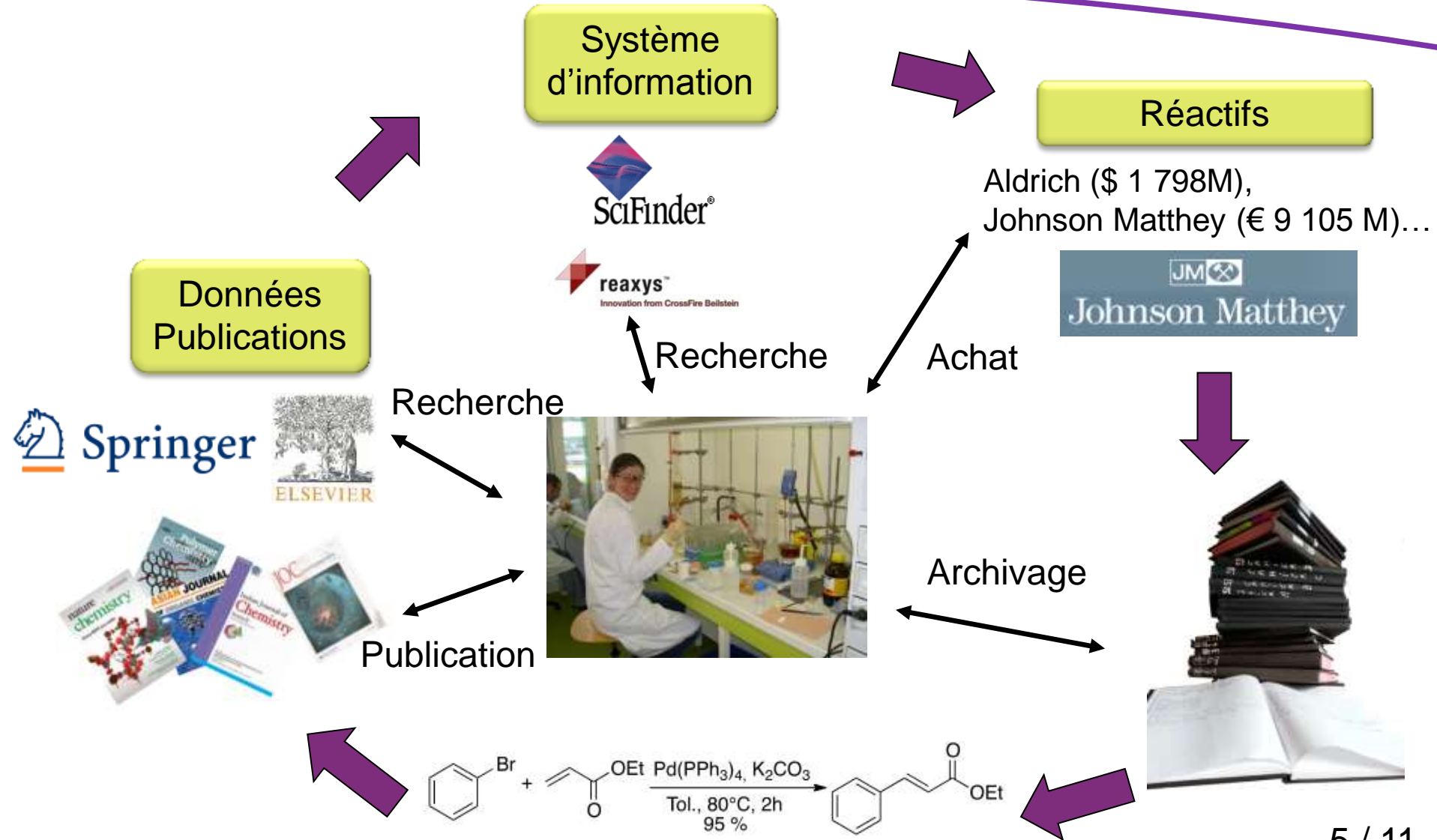
170 000 000 / year «lost chemistry»

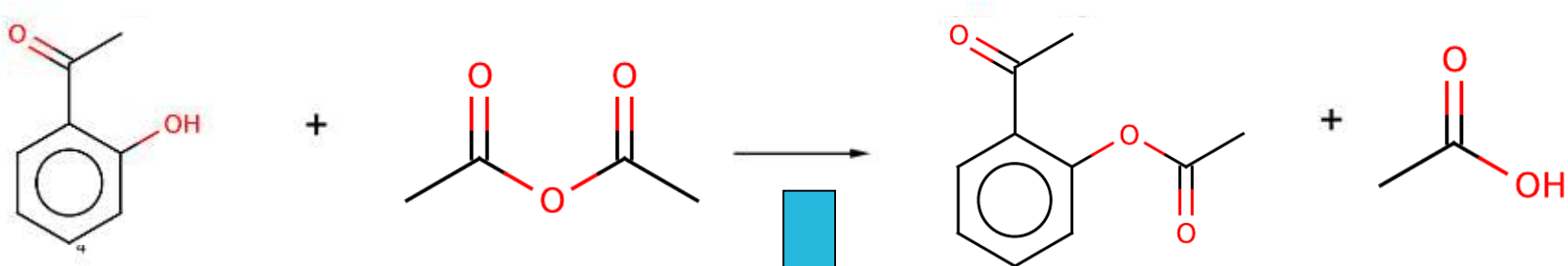
363. Labo

In scientific journals, only successful experiments are reported. But we should also report those that do not work. Due to lack of information, failed experiments are reproduced indefinitely by other scholars ignorant of their failure ...







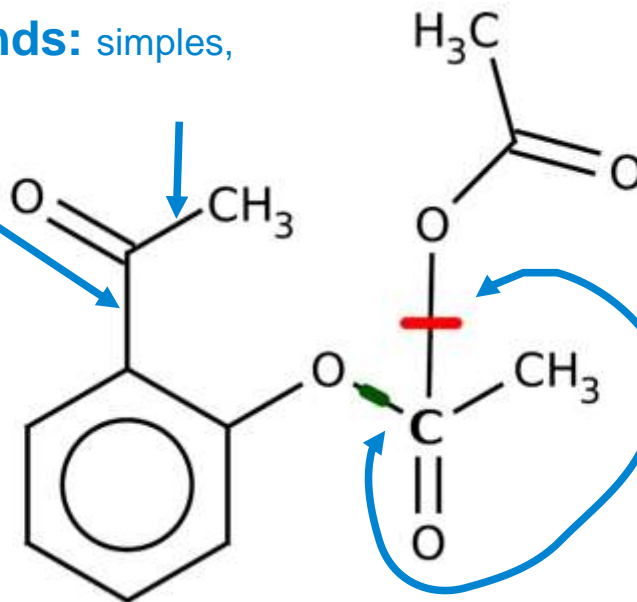


Transformation of a reaction into CGR

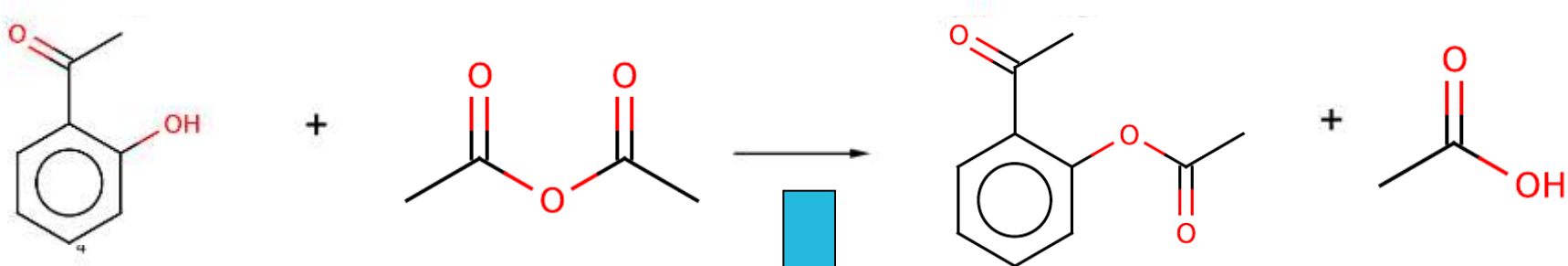
Conventional bonds: simples, doubles, aromatics ...



eSniff

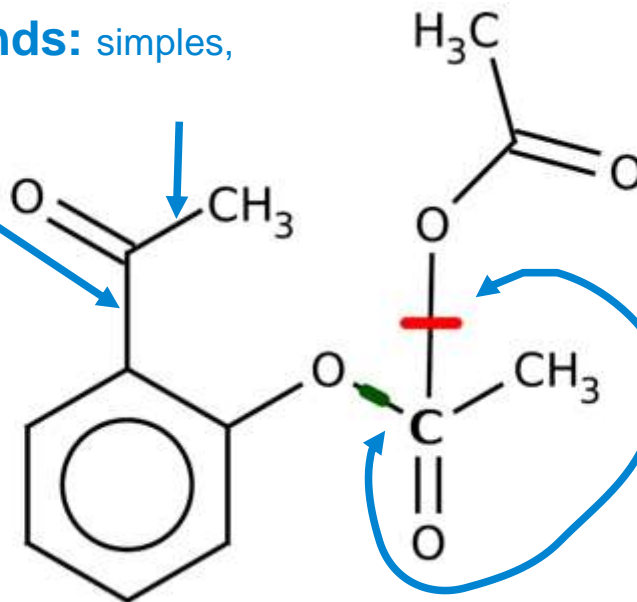


Dynamicals bonds:
Create a simple, break a simple, ...



Transformation of a reaction into
CGR

Conventional bonds: simples, doubles, aromatics ...



Dynamicals bonds:
Create a simple, break a simple, ...



Google for chemistry.

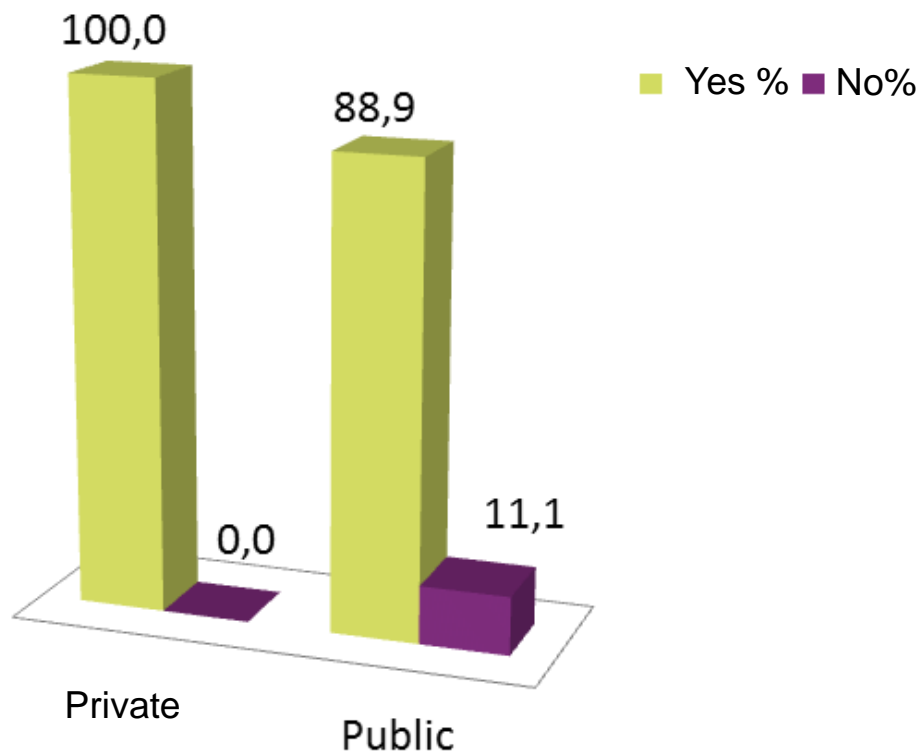
Similarity for reaction:

- Easier (draw what you need)
- Faster (one query -> find the best)
- Smarter (new knowledge)
- More relevant (think as a chemist)

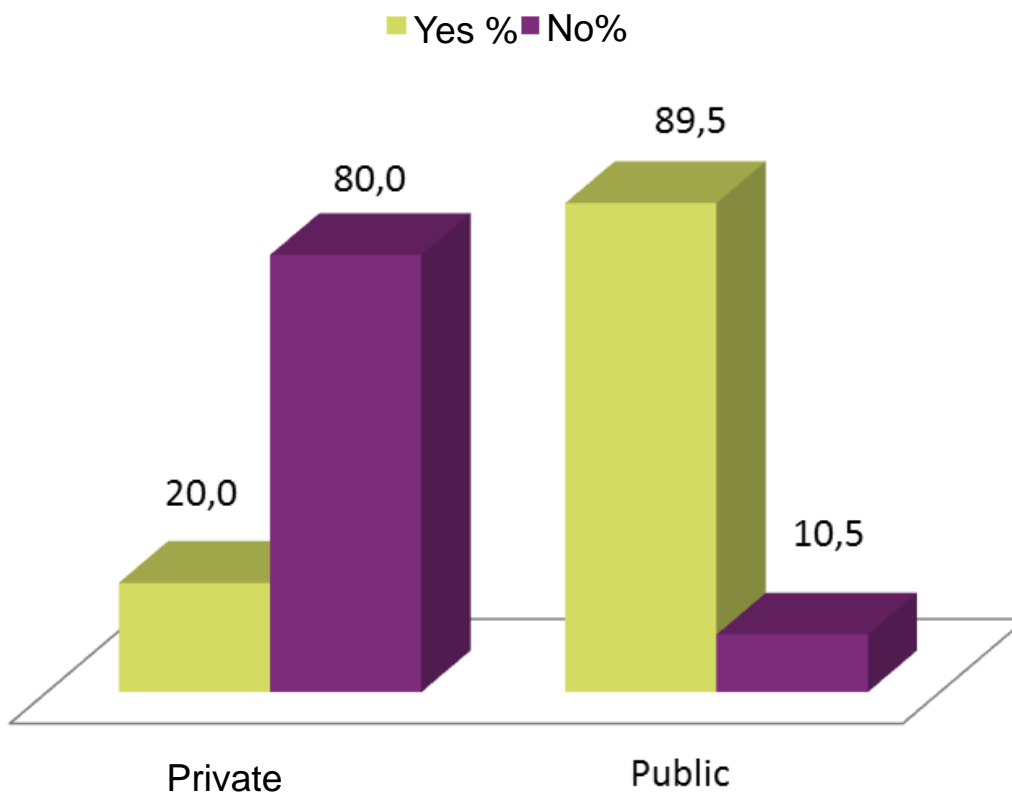
Use Failed reactions

- Anticipate side reactions
- Calculate protecting group stability

Would you be interested in using these data ?



Would you be interested in publishing data ?





Existing data in
Paper Notebook
(**ECLEIR** project)



Patent



eShare



PhD Thesis

Leader «lost Chemistry»

Today :

- 800 utilisateurs
- 1 000 000 réactions



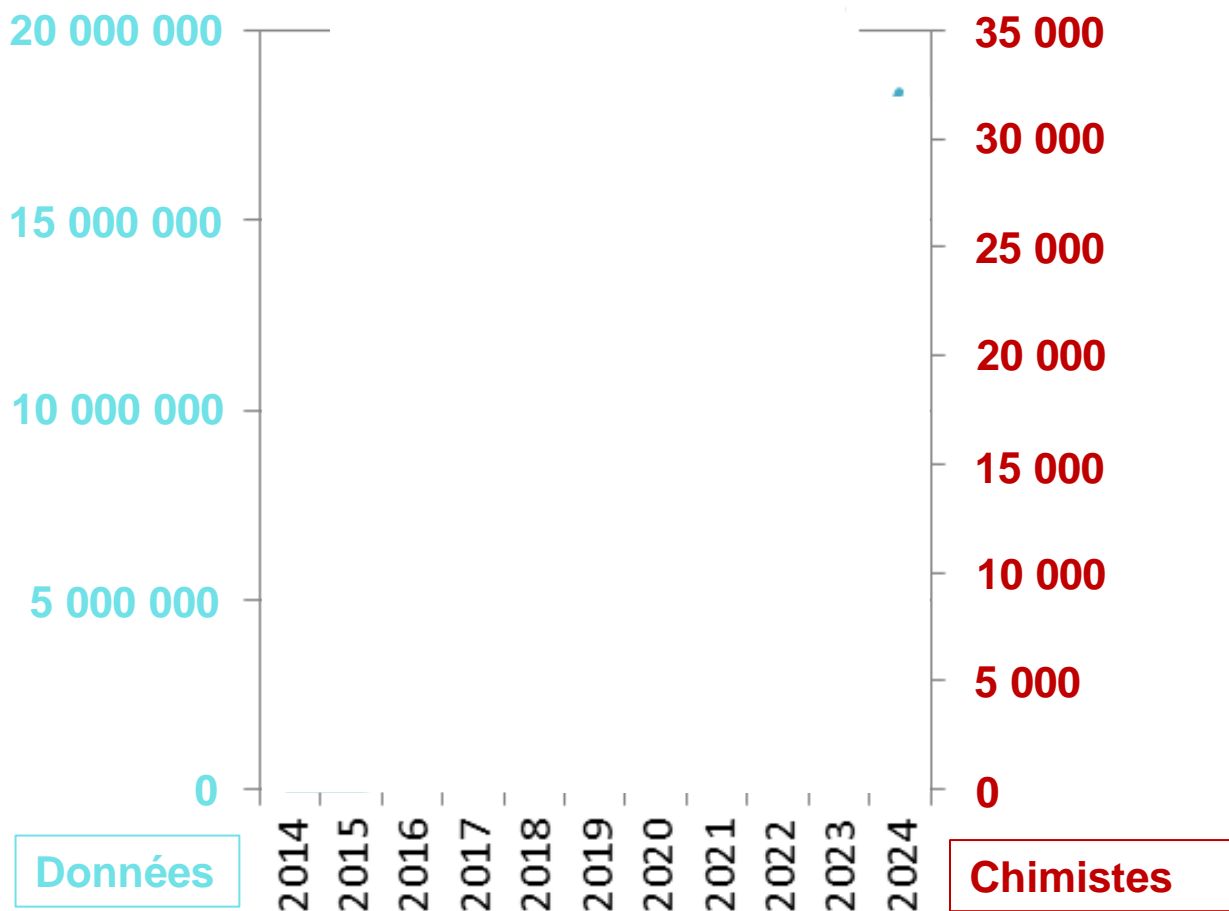
In 3 years :

- 6 500 utilisateurs
- 1 800 000 réactions

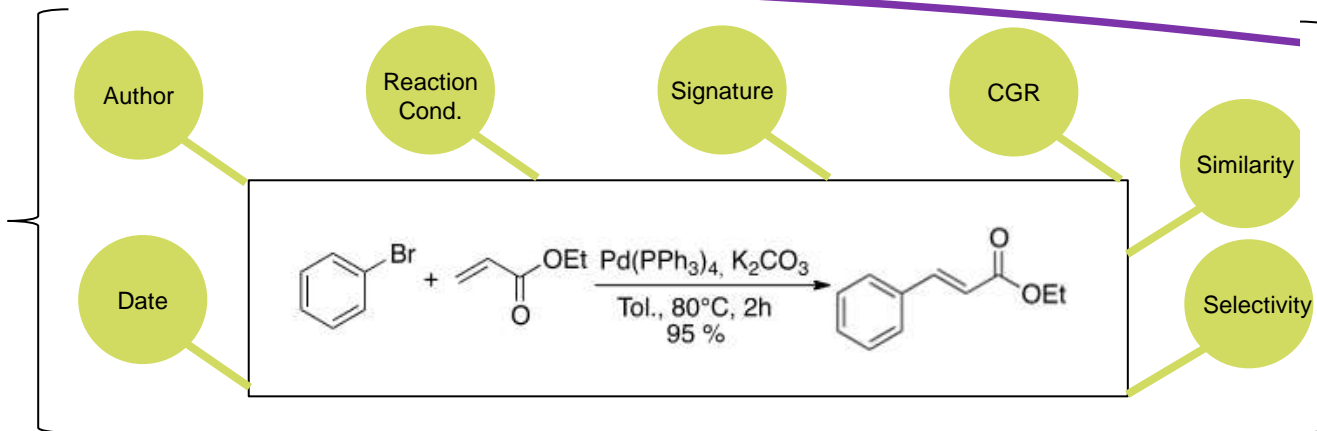


In 5 years :

- 10 400 utilisateurs ePro
- 2 500 000 réactions



Properties of reactions

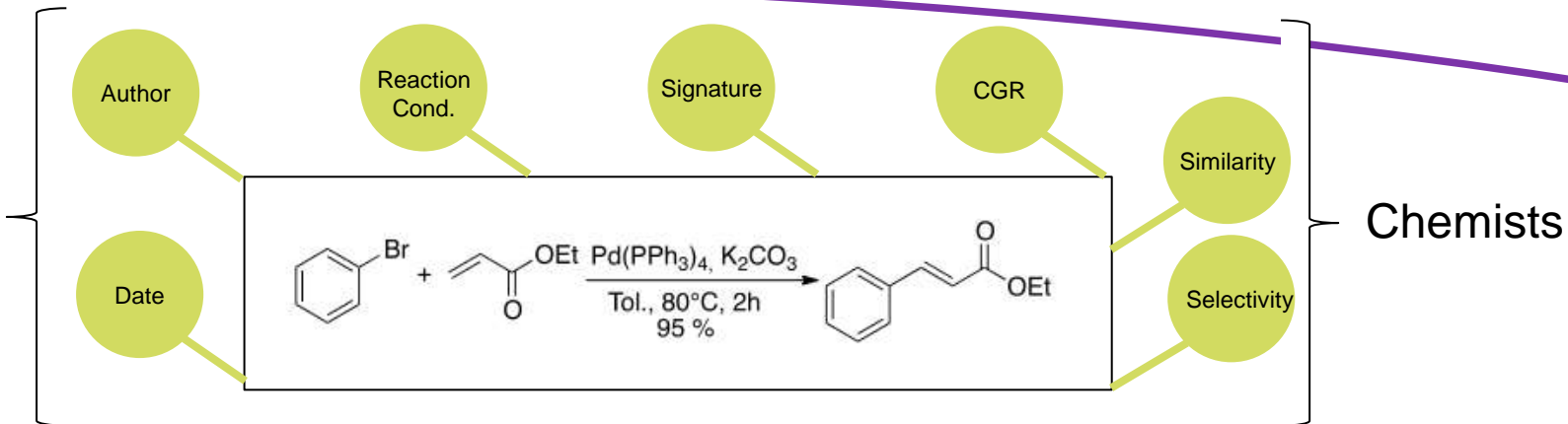


Chemists



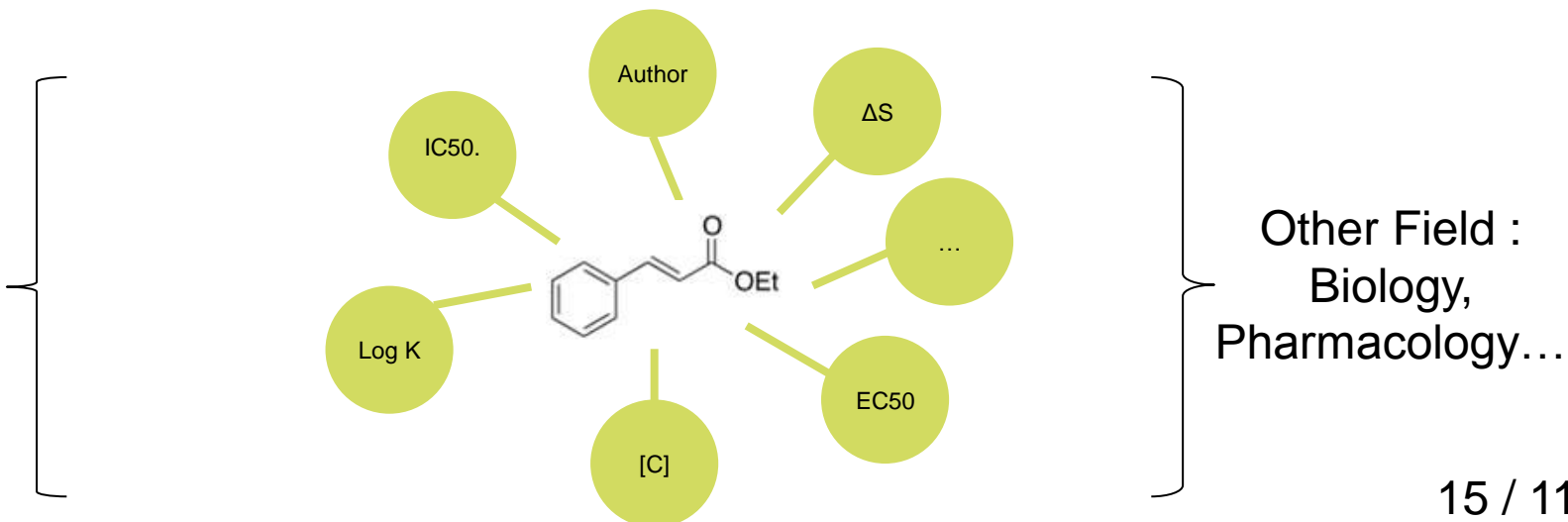
Tomorrow

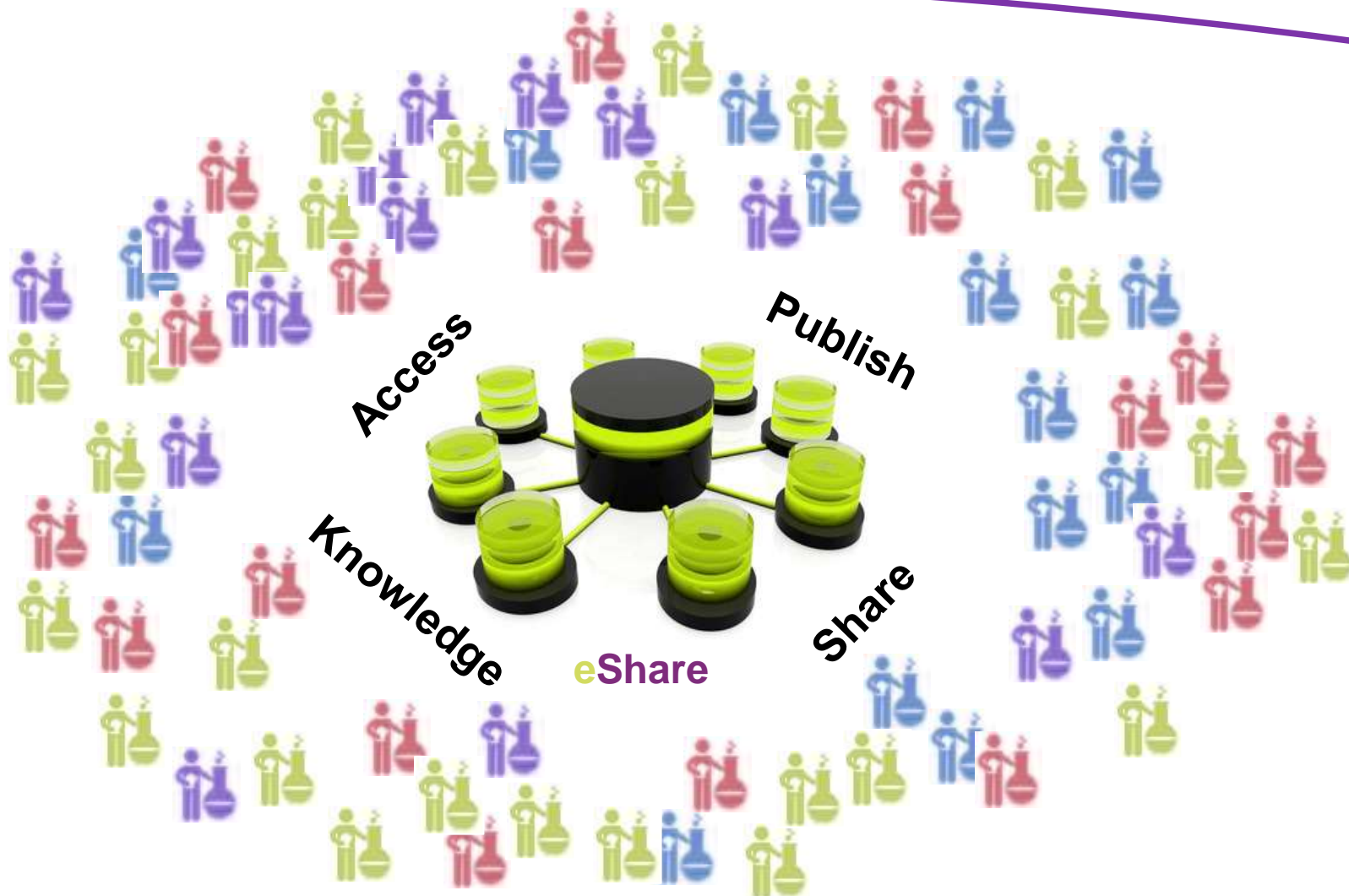
Properties of reactions



Tomorrow

Properties of compound





- Data existing, but are not easily accessible
- Both failed and successful experiment are needed
- Scientists agree to publish some of them, but need an easy way
- The more natural way is to use an ELN
- Laboratory notebook is the starting point for all knowledge...
- eNovalys propose an easy way from ELN to data Warehouse for the chemists and associate scientist.

Thank You

www.enovalys.com