

We devote all our knowledge
to serve people, enabling them
to lead long and healthy lives.

5 YEARS WITH CHEMAXON

Dancsó András

22 May 2019, ChemAxon UGM Budapest



A complex database

Chemical database technology:



Integration:



Programmers:

Pöcze Gábor
Uhrin Tamás
Vikár András
Peltz Csaba
Cseh Zoltán
Nyári Tibor

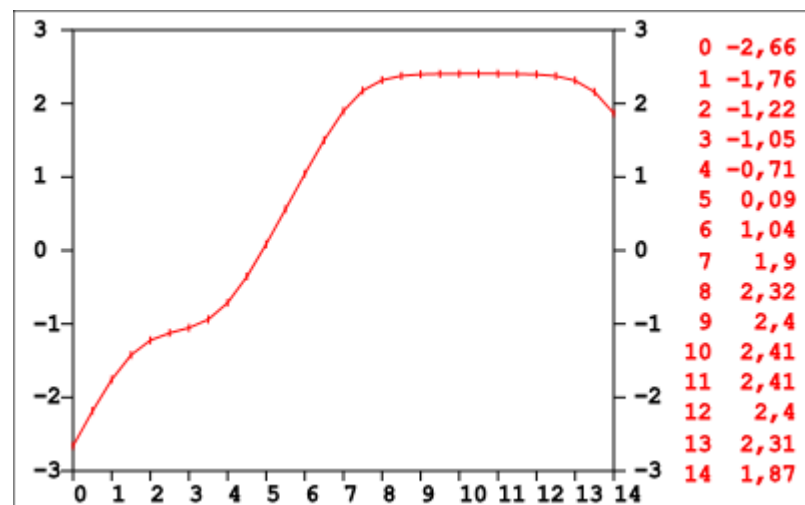
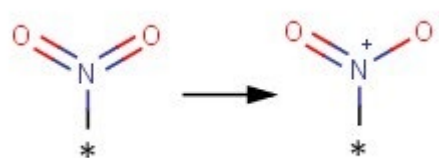
...

200 users:



ChemAxon components

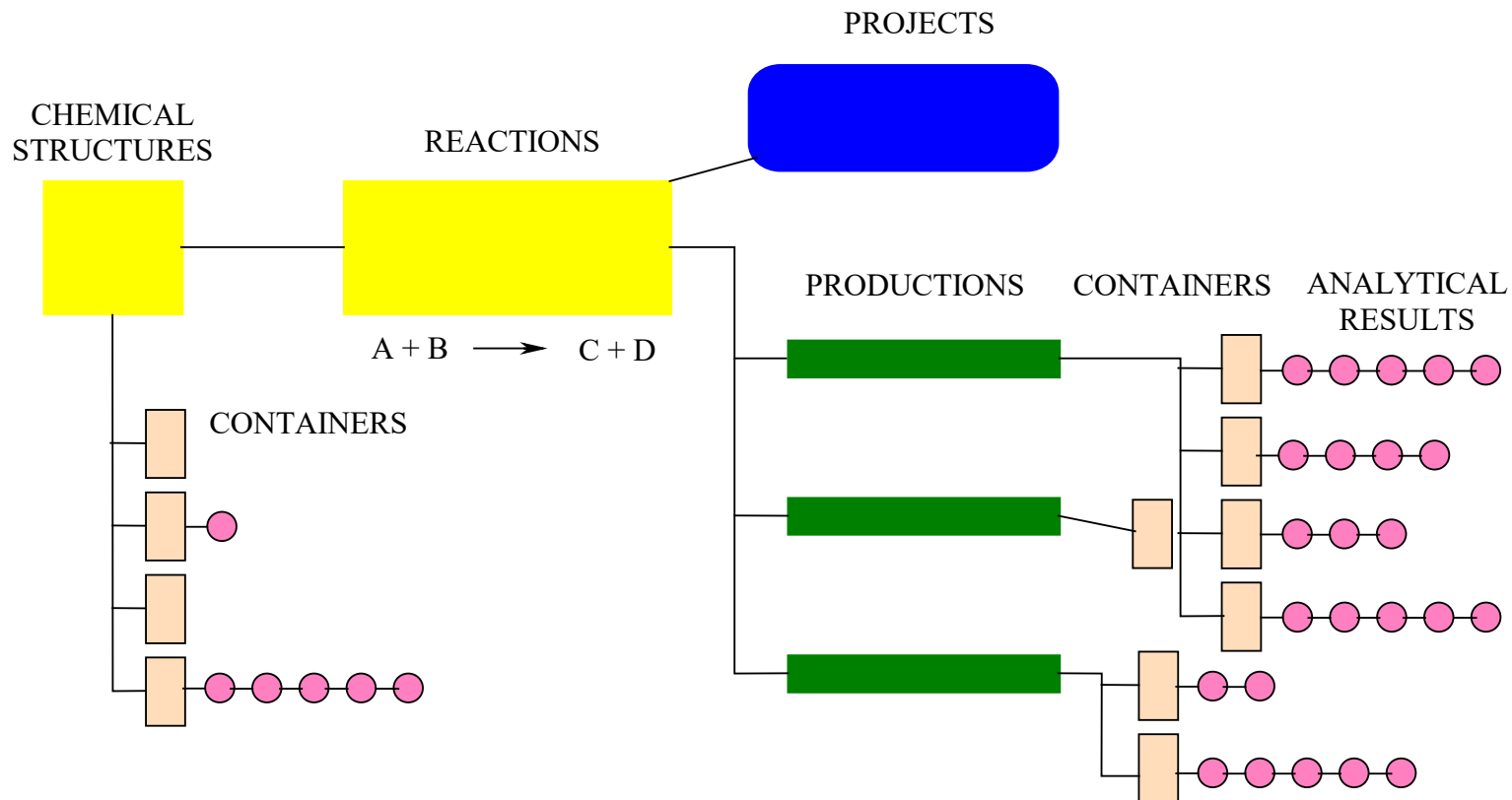
- JChem
- Marvin
- Marvin JS
- Standardizer
- Partitioning Plugin
- Structure to Name



Structure to Name

- Automatic name generation following registration or modification
- Successful in 99.8 %
- Exceptions: some rather complicated complexes, where even Reaxys didn't give a correct systematic name

Database structure



Logistics and ELN

Reagent containers:

- Unique barcode
- Location: building, room, cupboard, shelf, row
- Continuously tracked quantities

Safety:

- H and P phrases
- GHS symbols
- Label printing
- MSDS
- Controlled substances



§ Compliance Checker



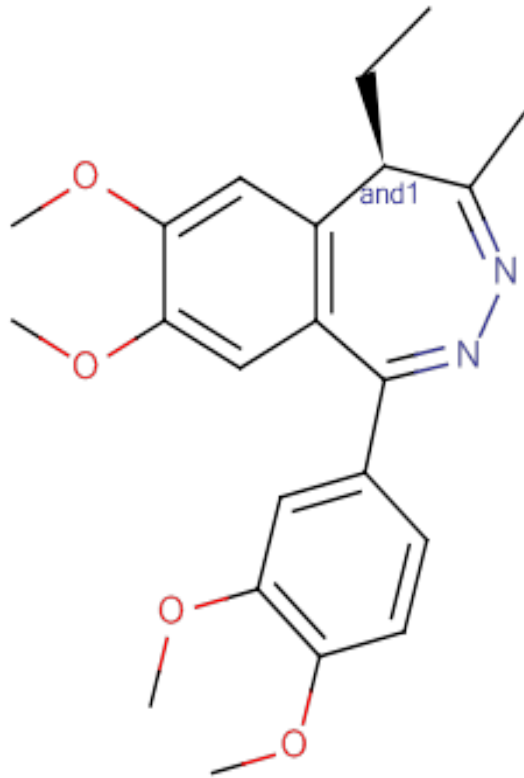
Procurement:

- Starting and tracking orders

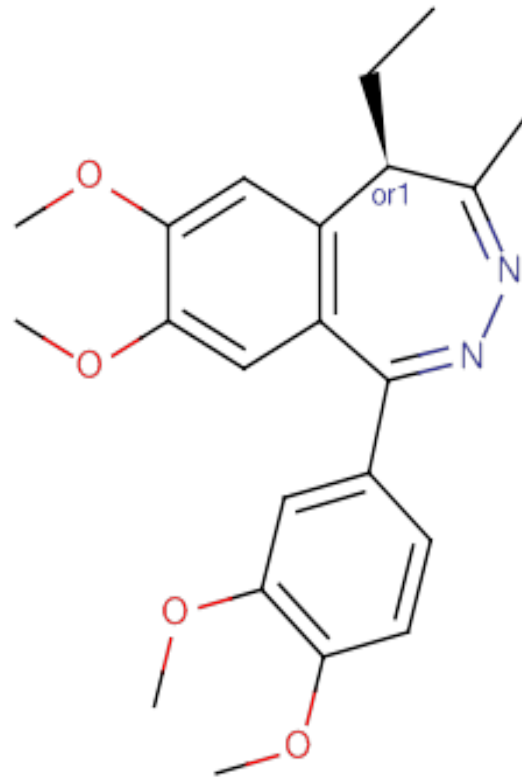
ELN functionality:

- Tracking of starting materials
- Physical constants
- Analytics
- Bilingual: English, Hungarian
- Hard copies

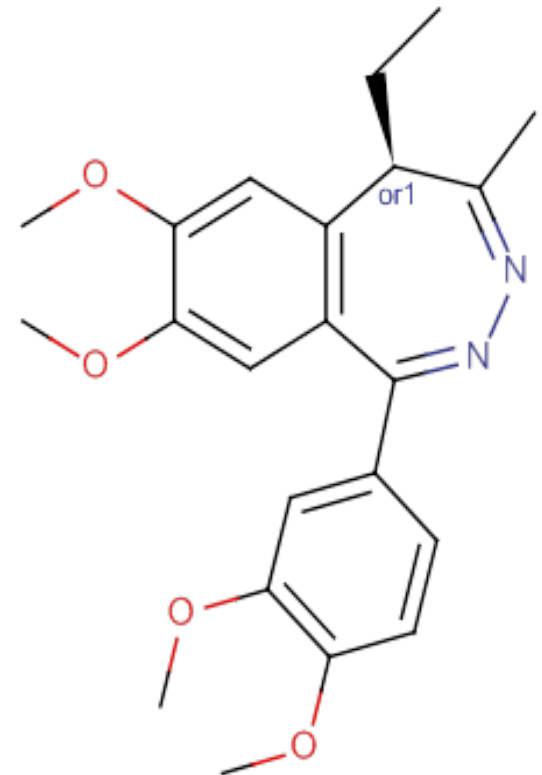
Stereochemistry



RACEMIC



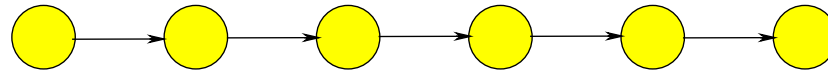
RESOLVED1



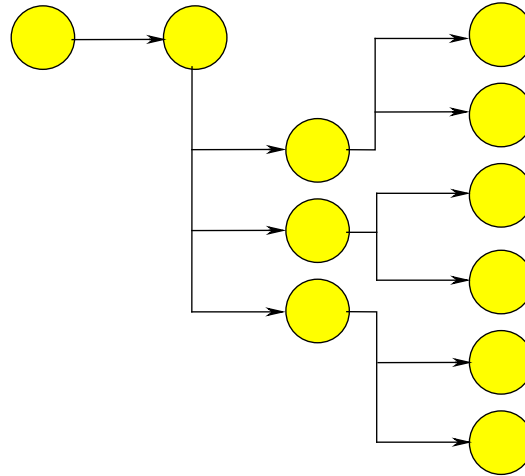
RESOLVED2

Example: tofisopam, an originality from Egis

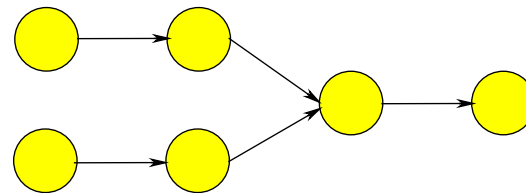
Synthesis schemes: basic types



Linear

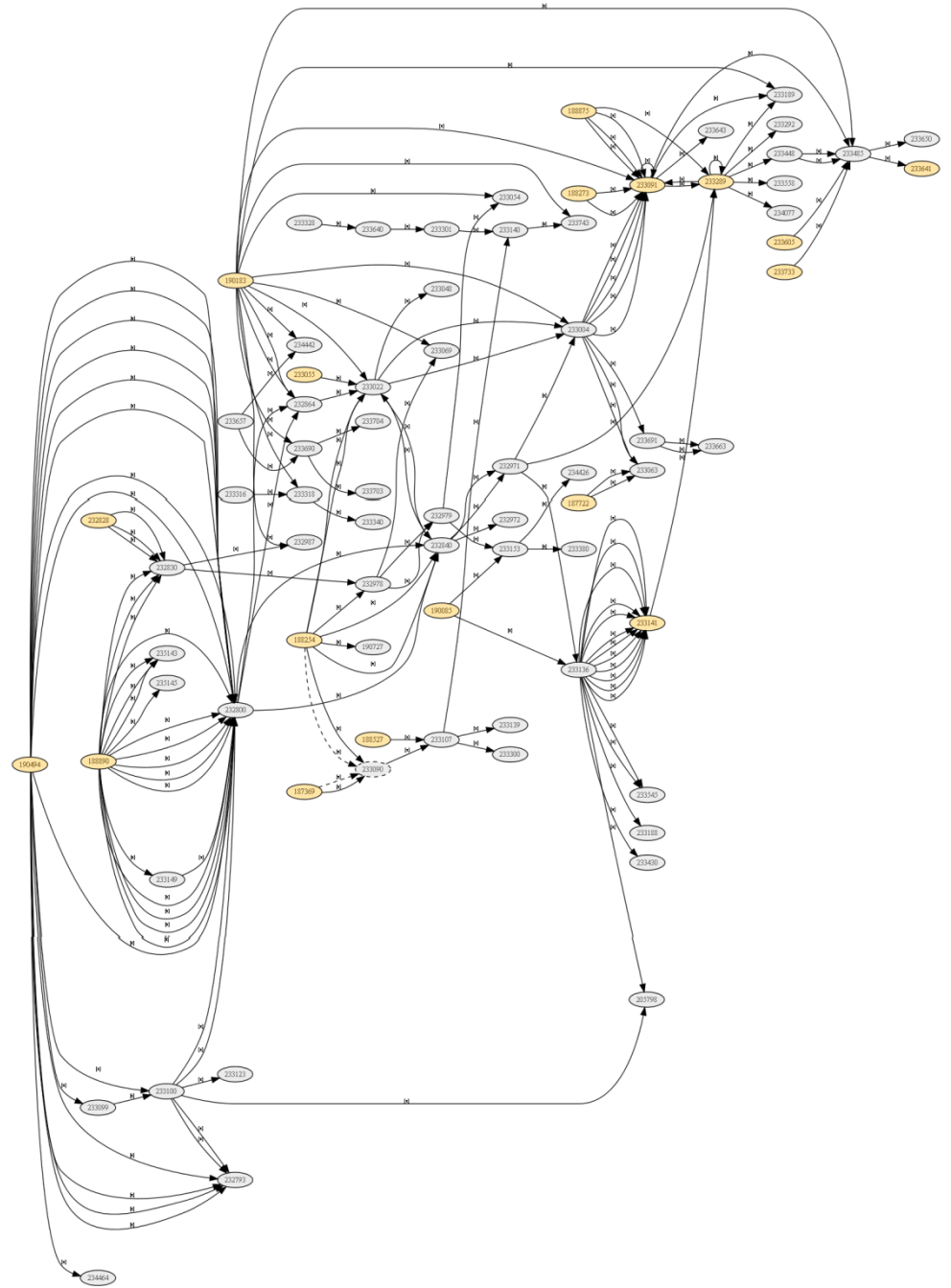


Combinatoric

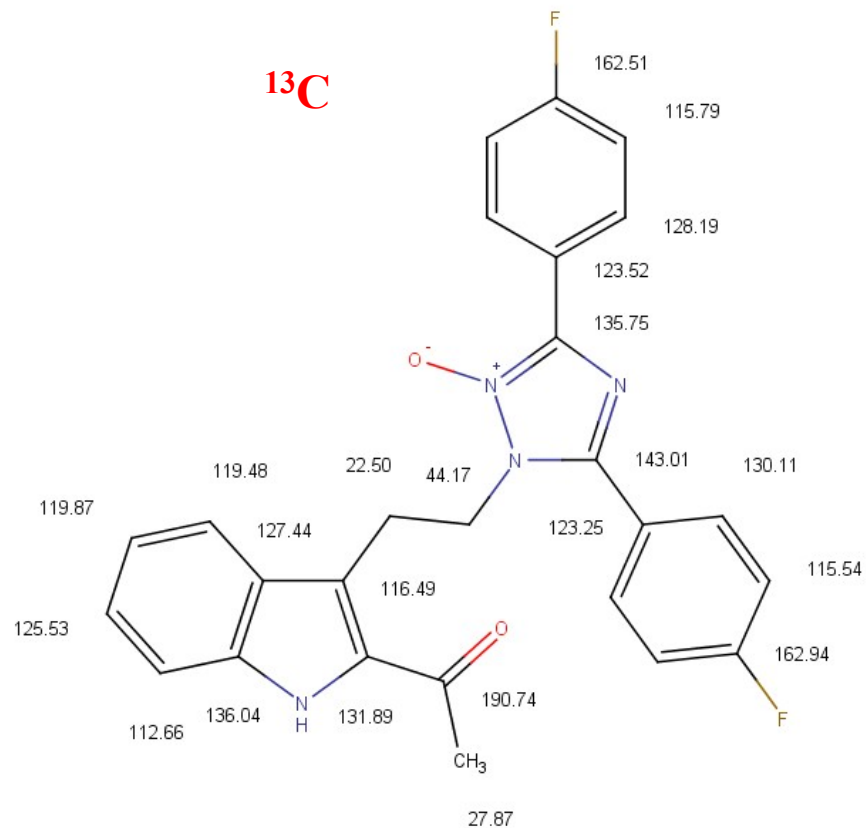
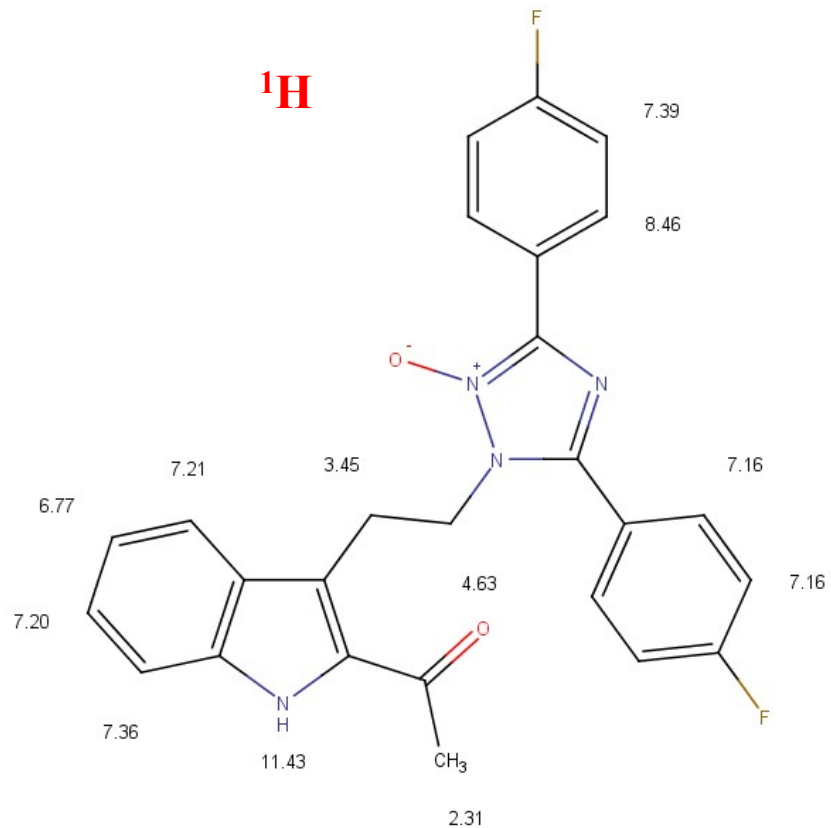


Convergent (Y)

Synthesis schemes: a real one



Assignment database



Milen, Matyas; Abranyi-Balogh, Peter; Dancso, Andras; Simig, Gyula; Keglevich, Gyorgy:

Reaction of 3,4-dihydro- β -carboline with 4-fluorophenyl-nitrile oxide, *Letters in Organic Chemistry*, **2010**, 7(5), 377-382.

Special thanks to

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IT project leaders:

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Vágó László
Nagy Szabolcs



Administration:

Simonyi Dalma

IT support:

Rétsági Péter
Kovács Róbert

200 users



Thank you for your attention!

