Storage and handling of structure and reaction information

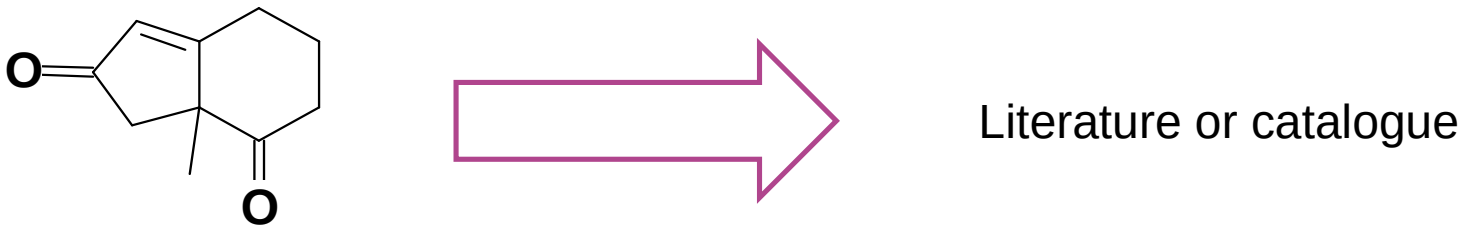
IC SYNTH

Chemisches Zentralblatt
Structural Database

Dr. Stephanie North

IC*SYNTH*: retrosynthesis planning tool concept

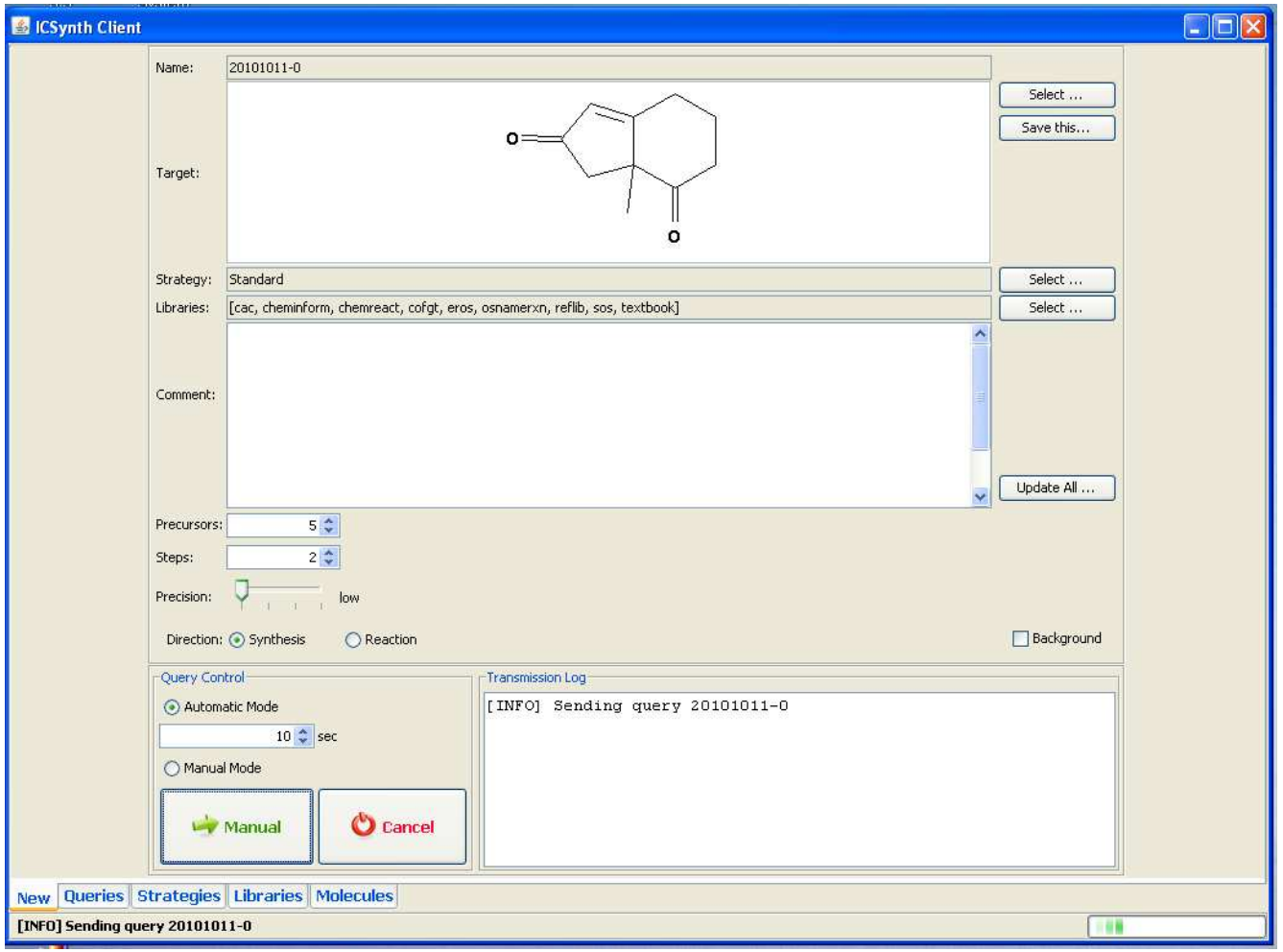
- Developed to facilitate chemists design synthetic pathways
  - How can I synthesize this target compound and what is the best strategy?
  - Are there any alternative approaches or reactions?



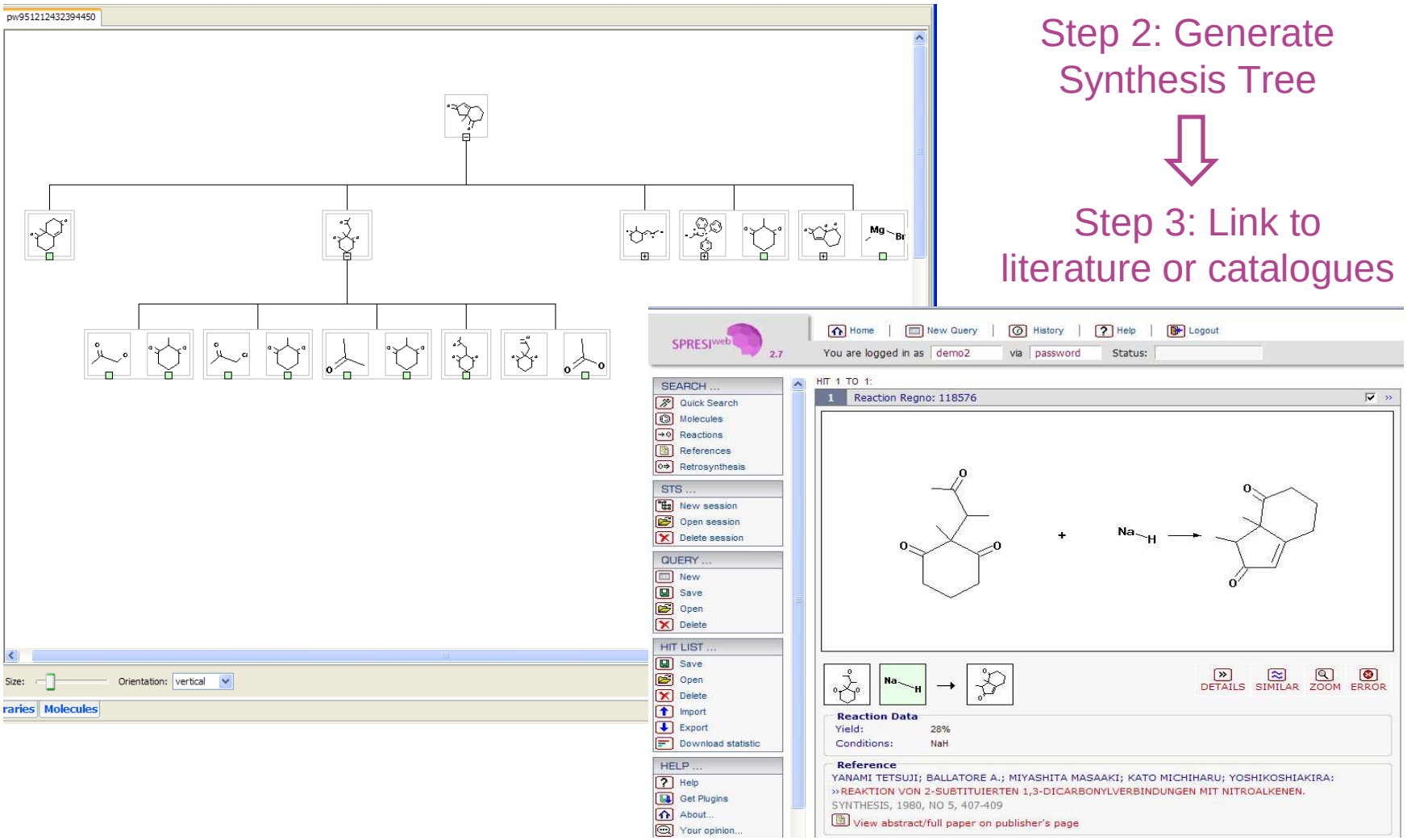
- IC*SYNTH* offers many advantages
- Based on published reactions from large data sources e.g. SPRESI, ChemInform
- Uses literature reaction databases to automatically generate transform libraries i.e. the knowledge base at the heart of IC*SYNTH*
- Can link to literature to verify the suggested reactions
- Check availability of precursors in commercial catalogues

IC*SYNTH:* intuitive, interactive synthesis design

Step 1: input target molecule



IC*SYNTH*: intuitive, interactive synthesis design



Step 2: Generate Synthesis Tree

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Step 3: Link to literature or catalogues

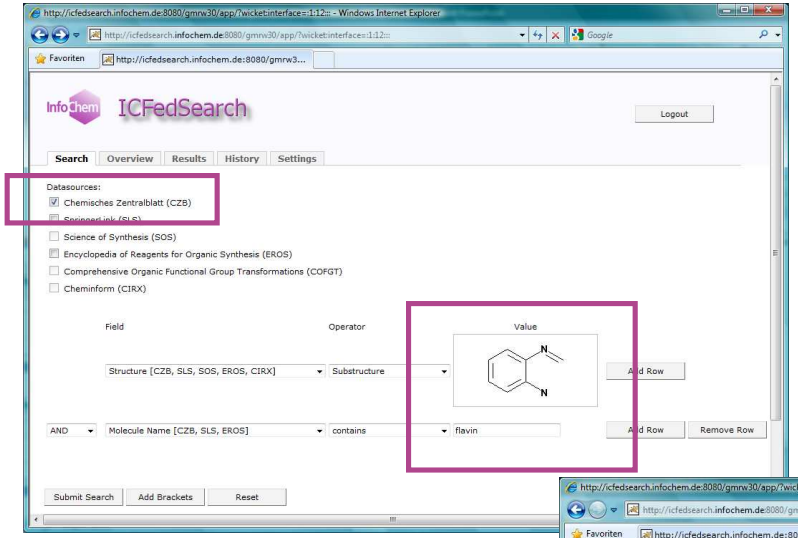
Chemisches Zentralblatt: new approach to historic source

- First and oldest abstracts journal in chemistry
- High quality abstracts covering literature from 1830 to 1969
  - Only abstracts journal before CA started in 1907
  - Complements Beilstein and Gmelin
- 900K pages, 1M unique names, 500K unique structures
- Relevant for prior art and freedom to operate, growing demand
- FIZ Chemie Berlin digitized CZB offering full text database
  - Abstracts in German with many old German chemical names
- InfoChem name to structure technology used to create a new CZB structure database
- Structures linked directly to text source resulting in a completely new way of searching CZB

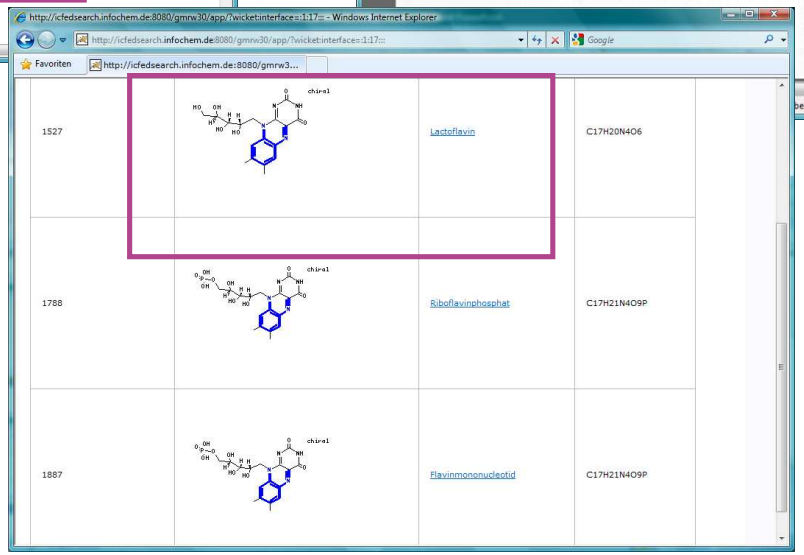

Pharmaceutisches
Central Blatt.
14. Januar 1830.
1.
Ankündigung.

First release on 1st November 2010

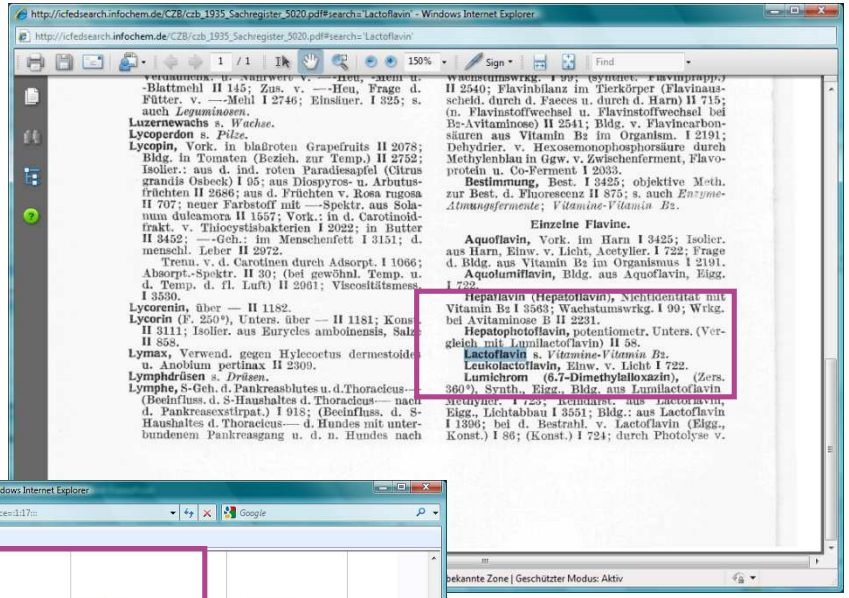
CZB structure searchable using ICFedSearch



Substructure and flavin



Lactoflavin



CZB abstract

Visit us at the InfoChem booth

IC SYNTH

Chemisches Zentralblatt Structural Database

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