



-7.3209	-1.0000	-0.4030	C
-9.9889	-0.1947	-0.3218	O
-10.2795	2.5700	0.1393	C
-8.5096	-1.8624	-0.6298	H
-7.5171	-2.3313	0.2921	H
-7.0177	-1.8762	-1.3207	H
-4.4781	1.2434	0.1858	C



Storage and handling
of **structure** and
reaction information



CHEMISCHES
ZENTRALBLATT
Structural Database



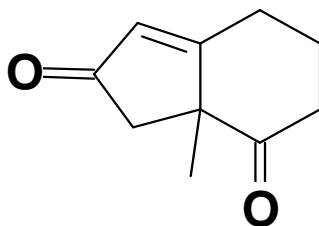
-7.3209	-1.0000	-0.4030	C
-9.9889	-0.1947	-0.3218	O
-10.2795	2.5700	0.1393	C
-8.5096	-1.8624	-0.6298	H
-7.5171	-2.3313	0.2921	H
-7.0177	-1.8762	-1.3207	H
-4.4781	1.2434	0.1858	C



2

ICSYNTH: 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?

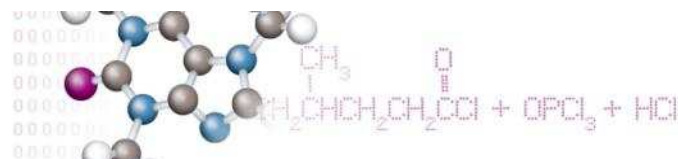


Literature or catalogue

- ICSYNTH 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 ICSYNTH
- Can link to literature to verify the suggested reactions
- Check availability of precursors in commercial catalogues



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-10.2795 2.5700 0.1393 C
-8.5096 -1.8624 -0.6298 H
-7.5171 -2.3313 0.2921 H
-7.0177 -1.8762 -1.3207 H
-4.4781 1.2434 0.1858 C



3

ICSYNTH: intuitive, interactive synthesis design

Step 1: input target molecule

The screenshot shows the ICSynth Client window with the following fields and controls:

- Name:** 20101011-0
- Target:** A chemical structure of a bicyclic molecule with a ketone group and a double bond.
- Strategy:** Standard
- Libraries:** [cac, cheminform, chemreact, cofgt, eros, osnamerxn, refileb, sos, textbook]
- Comment:** (Empty text area)
- Precursors:** 5
- Steps:** 2
- Precision:** low
- Direction:** Synthesis Reaction
- Background:**
- Query Control:** Automatic Mode (10 sec), Manual Mode
- Transmission Log:** [INFO] Sending query 20101011-0
- Buttons:** Select..., Save this..., Update All..., Manual, Cancel

At the bottom, there are tabs for New, Queries, Strategies, Libraries, and Molecules, and a status bar showing [INFO] Sending query 20101011-0.

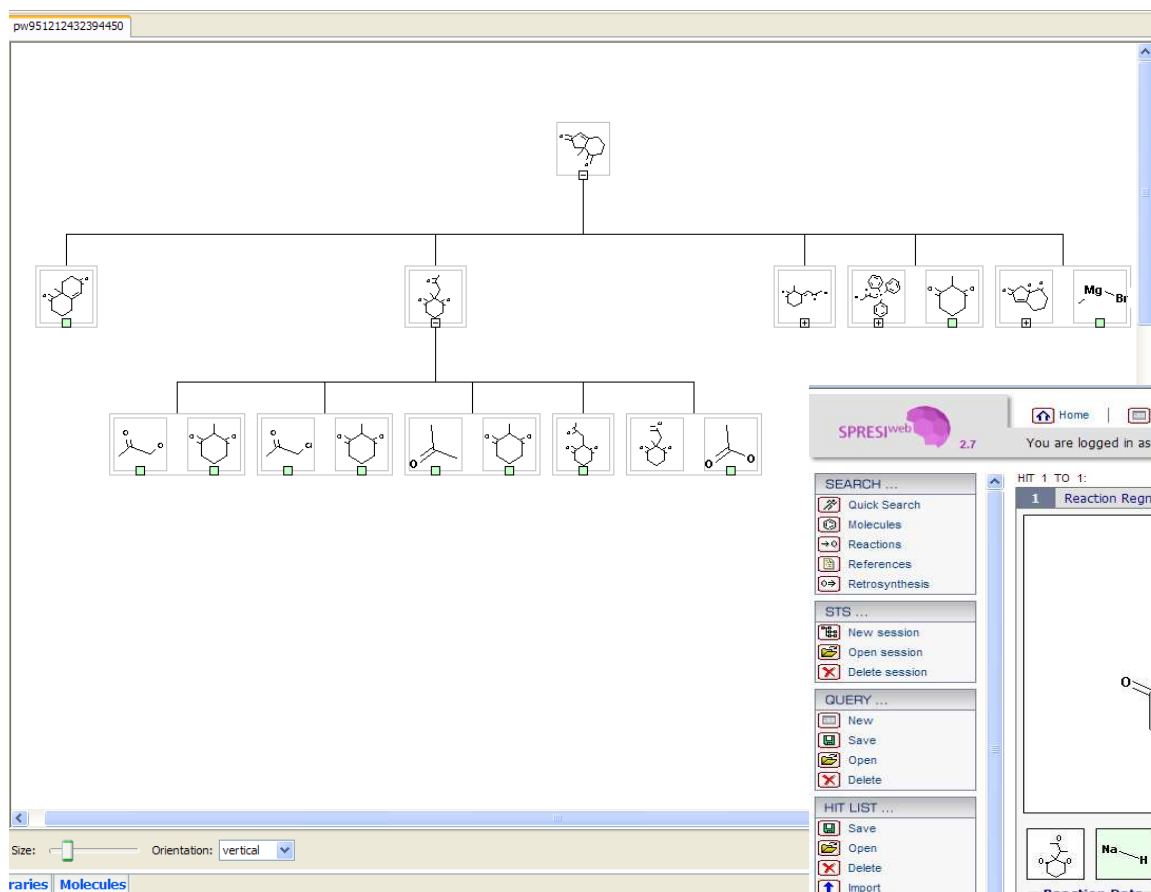


-7.3209 -1.0000 -0.4030 C
-9.9889 -0.1947 -0.3218 O
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-7.0177 -1.8762 -1.3207 H
-4.4781 1.2434 0.1858 C



4

ICSYNTH: intuitive, interactive synthesis design



Step 2: Generate
Synthesis Tree



Step 3: Link to
literature or catalogues

SPRESJweb 2.7

Home | New Query | History | Help | Logout

You are logged in as demo2 via password Status:

HIT 1 TO 1:
1 Reaction Regno: 118576

Reaction: CC1(C)C(=O)C2(C)C(=O)C1C2 + Na-H >> CC1(C)C(=O)C2(C)C=C1C2

Reaction Data
Yield: 28%
Conditions: NaH

Reference
YANAMI TETSUJI; BALLATORE A.; MIYASHITA MASAOKI; KATO MICHIHARU; YOSHIKOSHIKIRA:
>>REAKTION VON 2-SUBSTITUIERTEN 1,3-DICARBONYLVERBINDUNGEN MIT NITROALKENEN.
SYNTHESIS, 1980, NO 5, 407-409
[View abstract/full paper on publisher's page](#)



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CHEMISCHES
ZENTRALBLATT
Structural Database



5

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



First release on 1st November 2010



-7.2209 -1.0000 -0.4030 C
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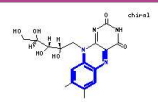




CZB structure searchable using ICFedSearch

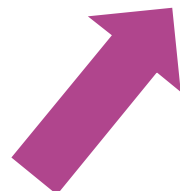
Substructure and flavin



Lactoflavin

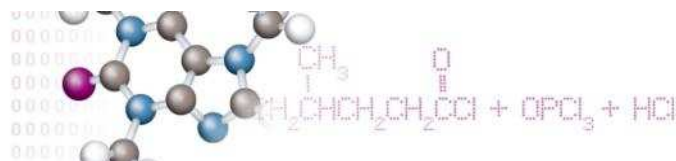
1527		Lactoflavin	C17H20N4O6
1788		Riboflavinphosphat	C17H21N4O9P
1887		Flavinmononucleotid	C17H21N4O9P

CZB abstract





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7

Visit us at the InfoChem booth



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InfoChem GmbH: www.infochem.de, www.spresi.com, info@infochem.de