MISSIONE 4
ISTRUZIONE
RICERCA

Finanziato dall'Unione europea
NextGenerationEU

Ministero dell'Università e della Ricerca

Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

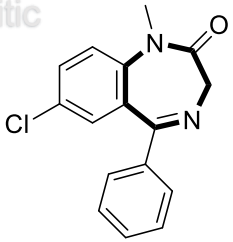
UniUrb_Hetslab: a unique virtual library for computational hit identification

Università degli Studi di Urbino
23 maggio 2024

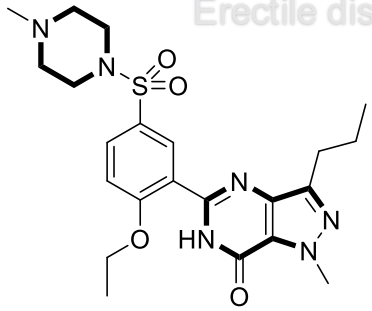
HETEROCYCLES

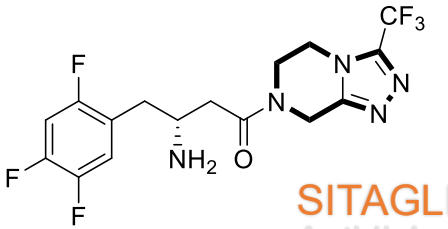
PHARMACEUTICAL

DIAZEPAM
Anxiolitic



SILDENAFIL
Erectile disfunctions

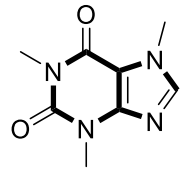




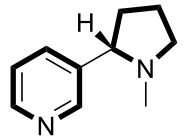
SITAGLIPTIN
Antidiabetic

NATURAL COMPOUNDS

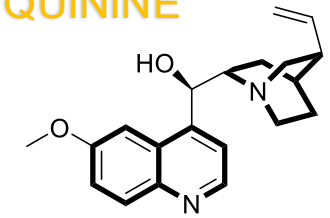
CAFFEIN



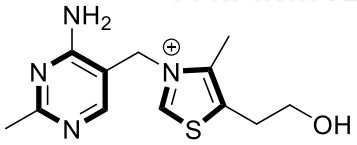
NICOTINE



QUININE



THIAMINE



Dott.ssa
De Crescentini

Prof.
Favi

Dott.ssa
Santeusanio

Prof.
Mantellini

Dott.ssa
Caselli

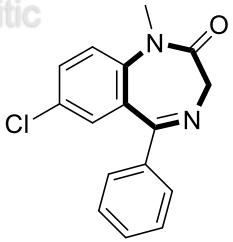
Dott.
Ciccone

Dott.
Mari

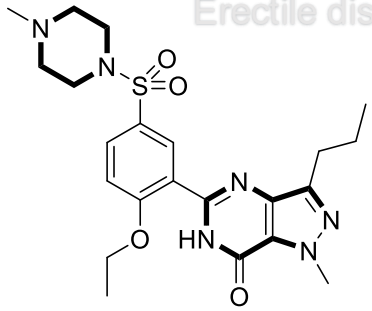
HETEROCYCLES

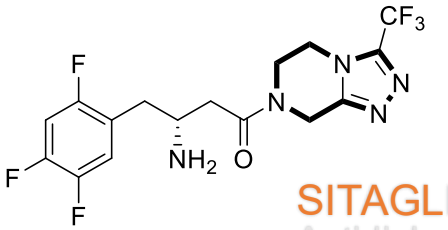
PHARMACEUTICAL

DIAZEPAM
Anxiolitic

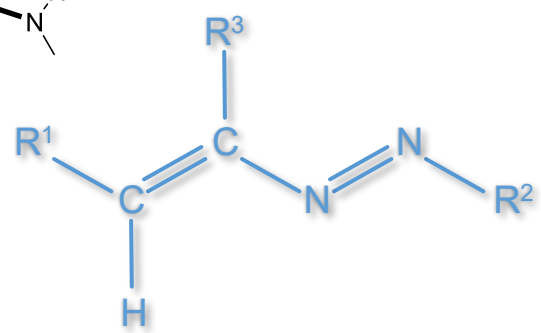


SILDENAFIL
Erectile disfunctions



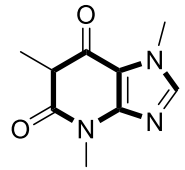


SITAGLIPTIN
Antidiabetic

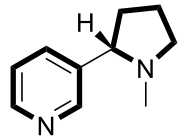


NATURAL COMPOUNDS

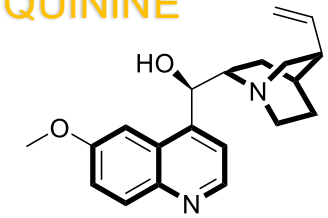
CAFFEIN



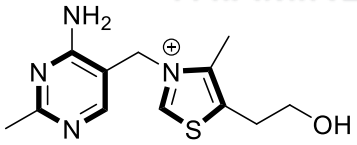
NICOTINE



QUININE



THIAMINE



Dott.ssa De Crescentini

Prof. Favi

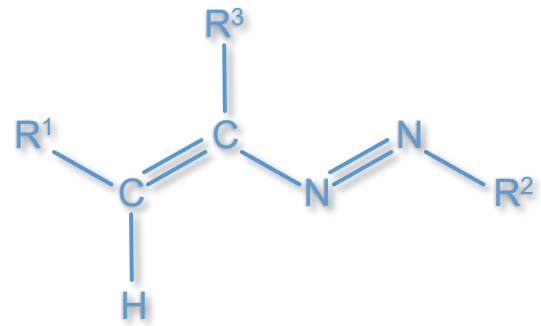
Dott.ssa Santeusanio

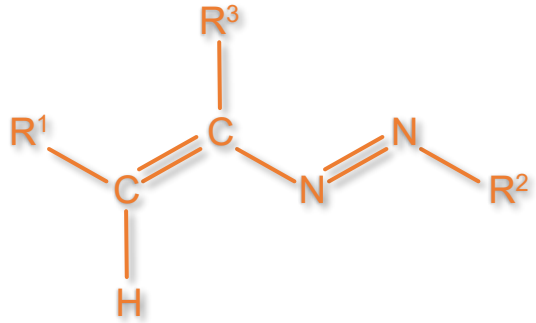
Prof. Mantellini

Dott.ssa Caselli

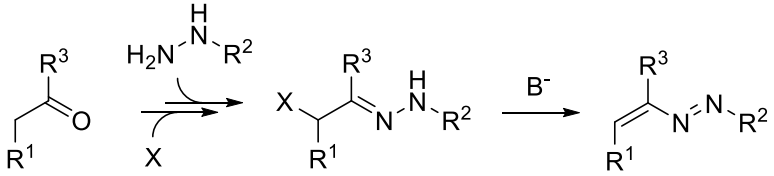
Dott. Ciccone

Dott. Mari

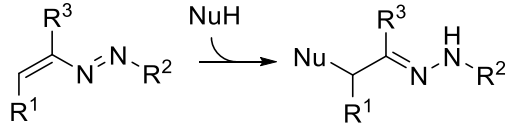

R3
R1
C
N
N
R2
C
H



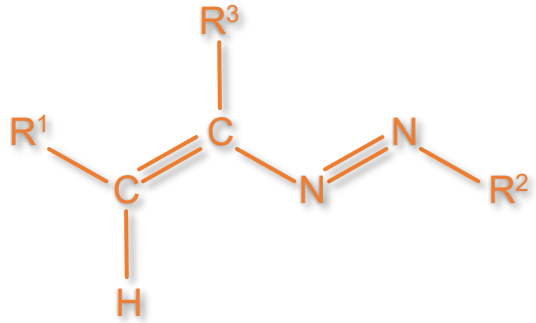
SYNTHESIS



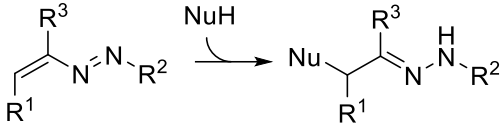
REACTIVITY

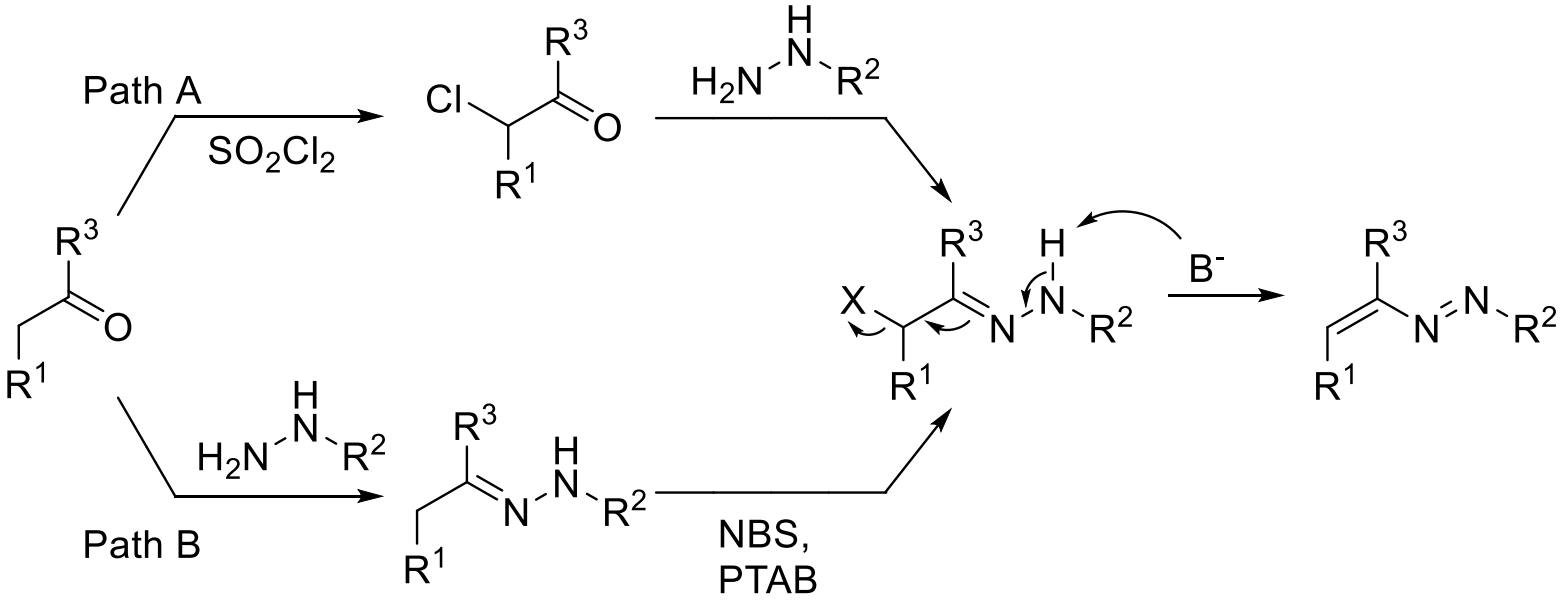


SYNTHESIS

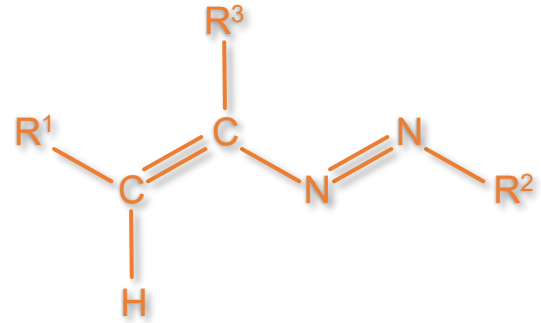


REACTIVITY

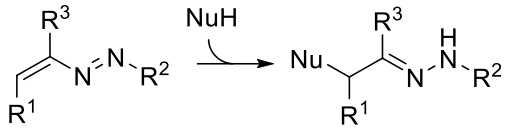


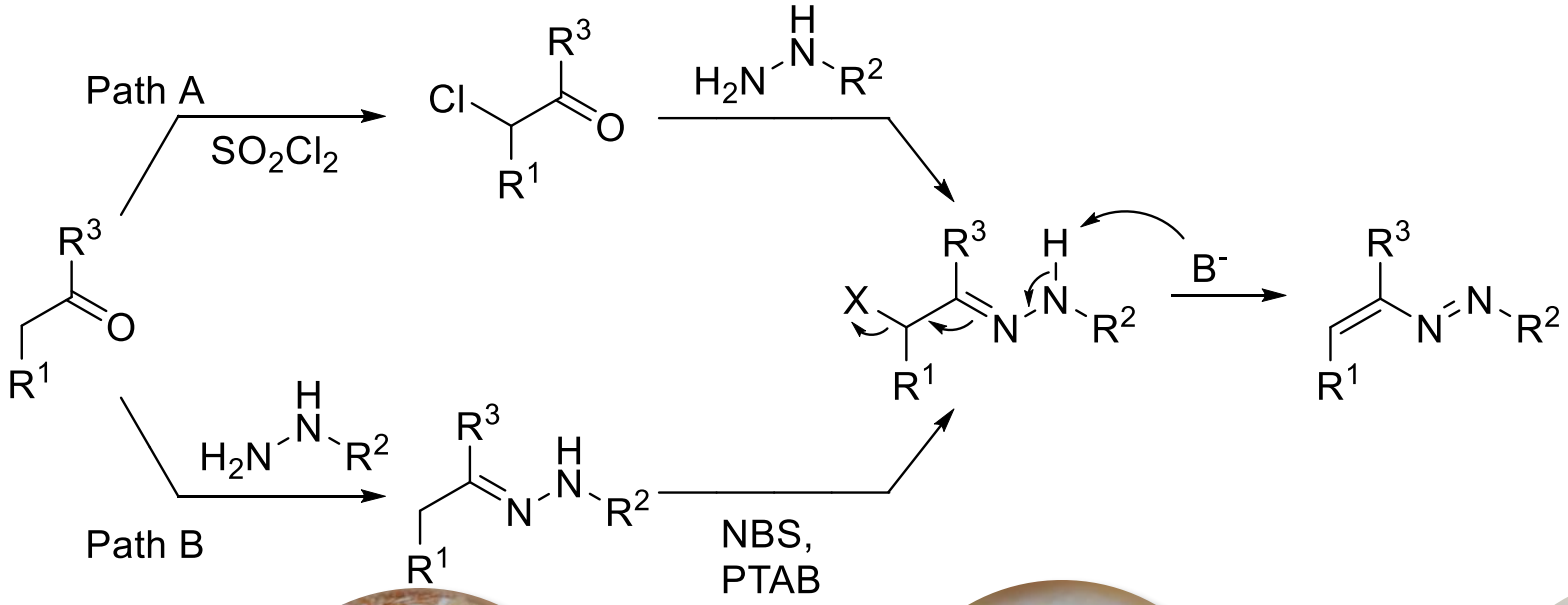


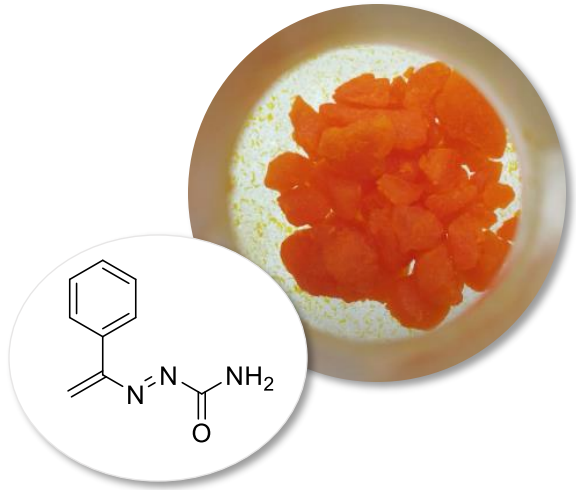
SYNTHESIS

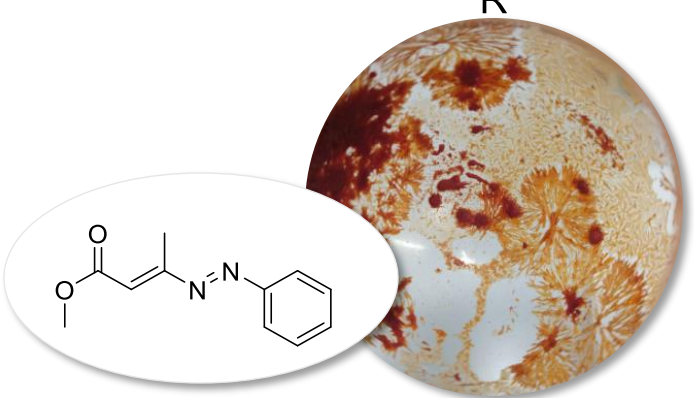


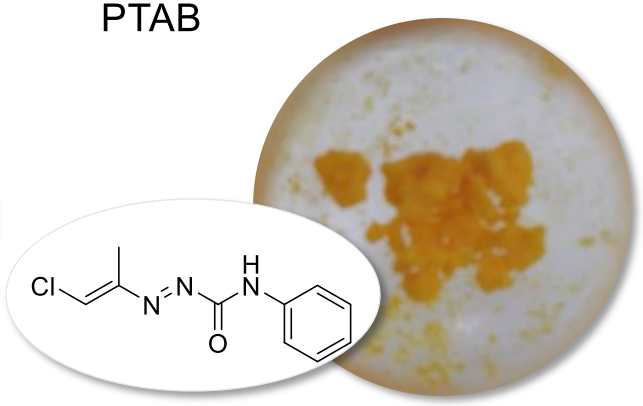
REACTIVITY

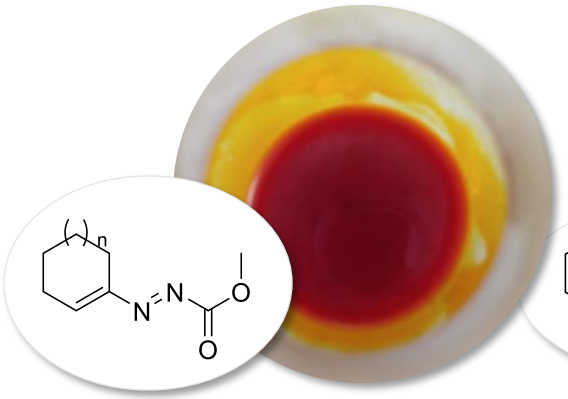


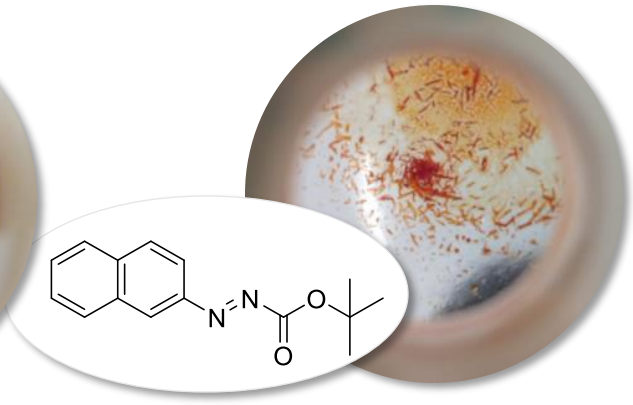


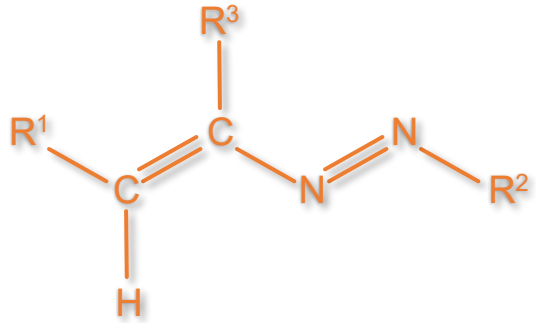




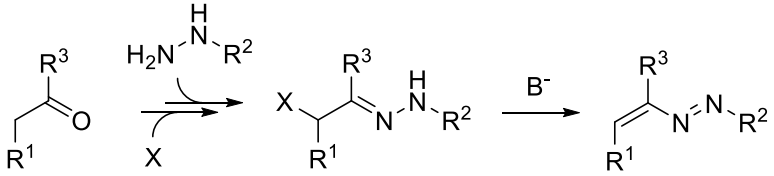




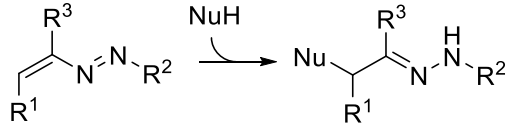




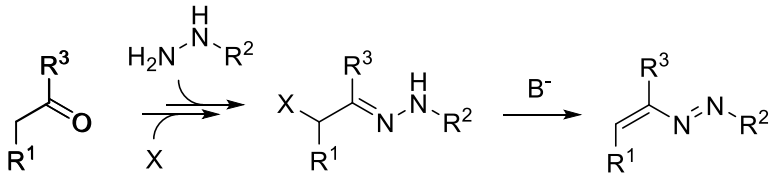
SYNTHESIS

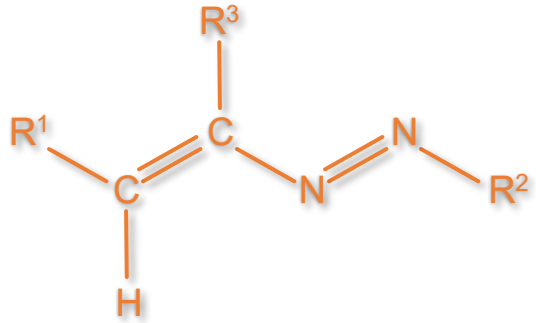


REACTIVITY

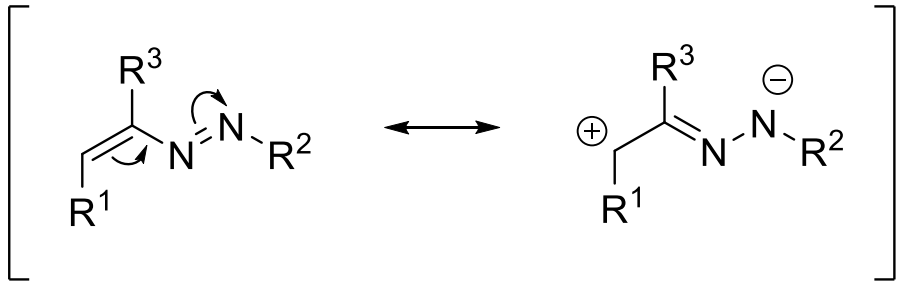


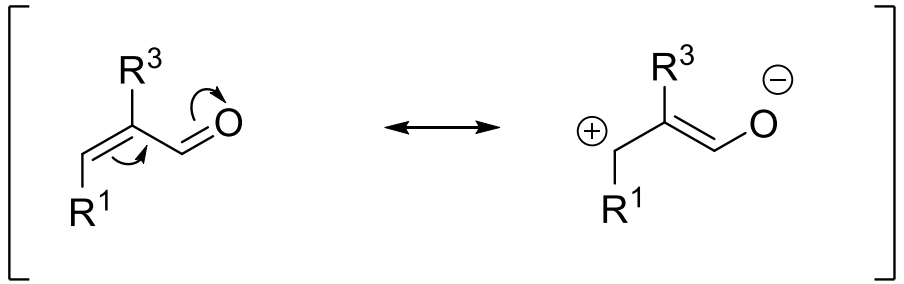
SYNTHESIS



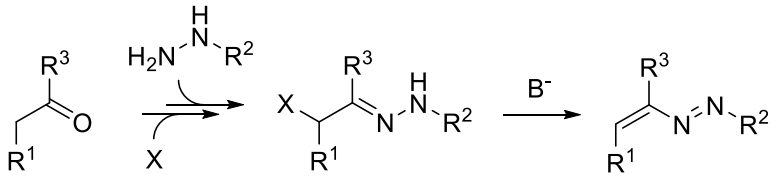


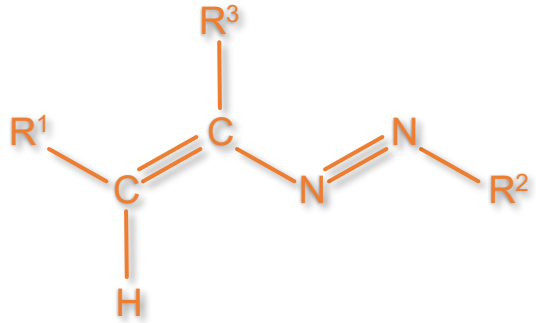
REACTIVITY



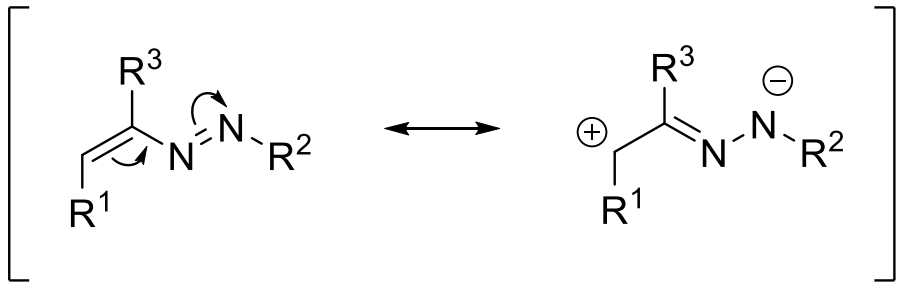


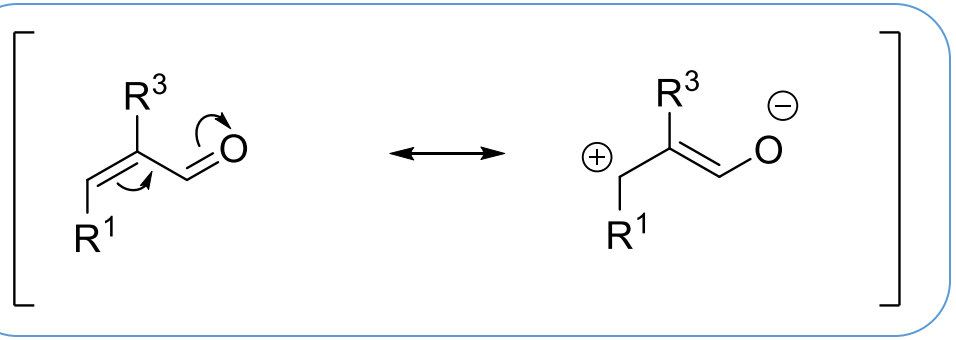
SYNTHESIS

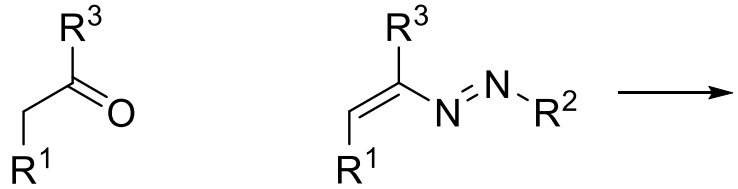




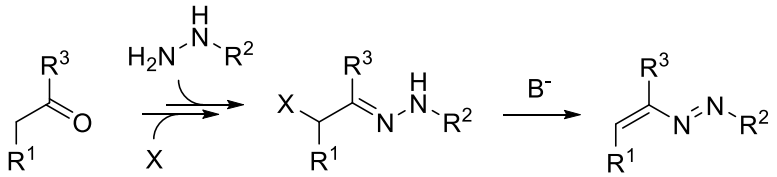
REACTIVITY

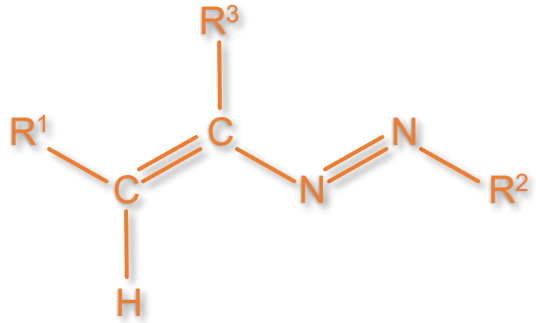




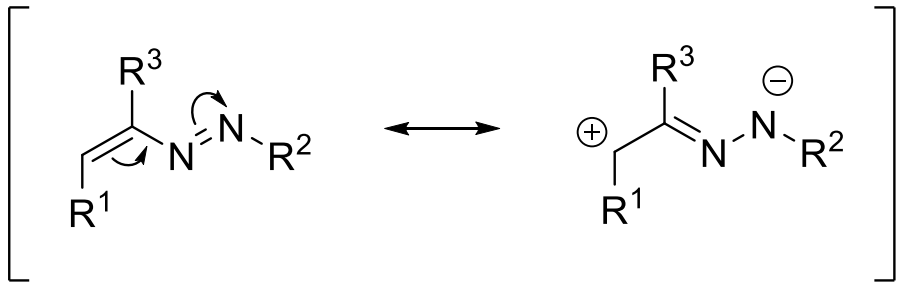


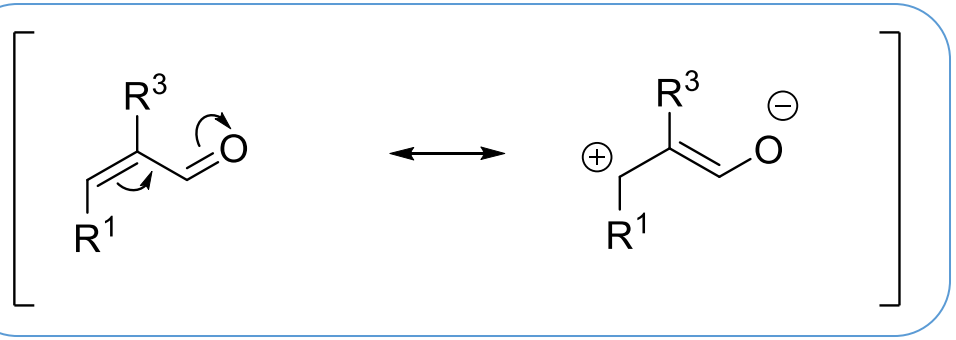
SYNTHESIS

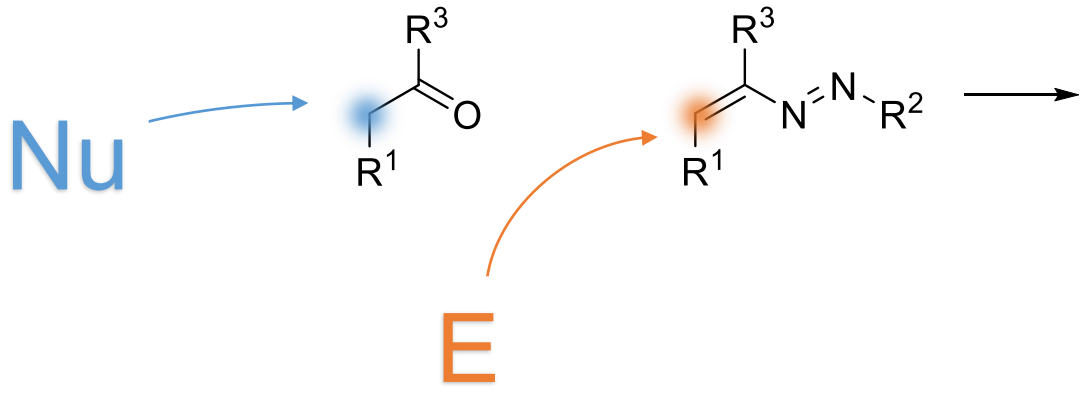




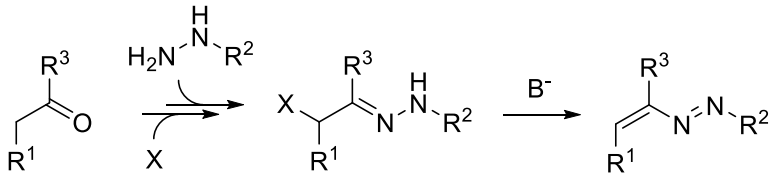
REACTIVITY

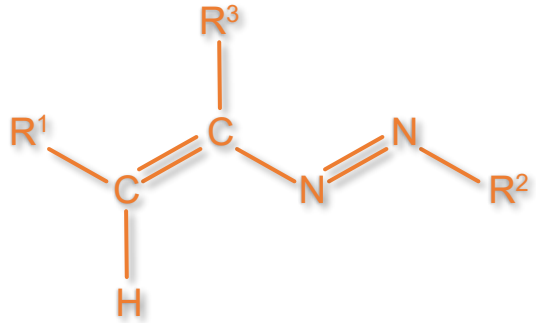




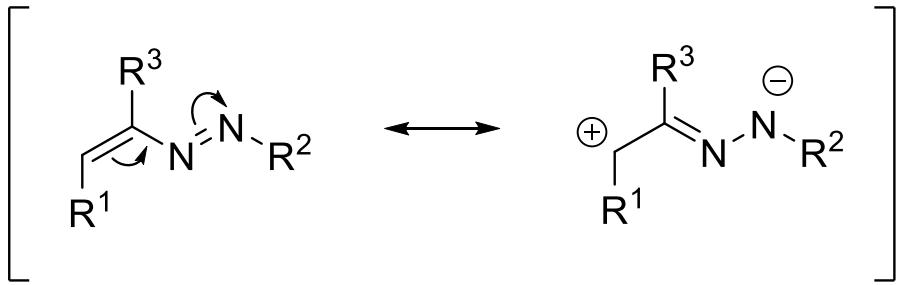


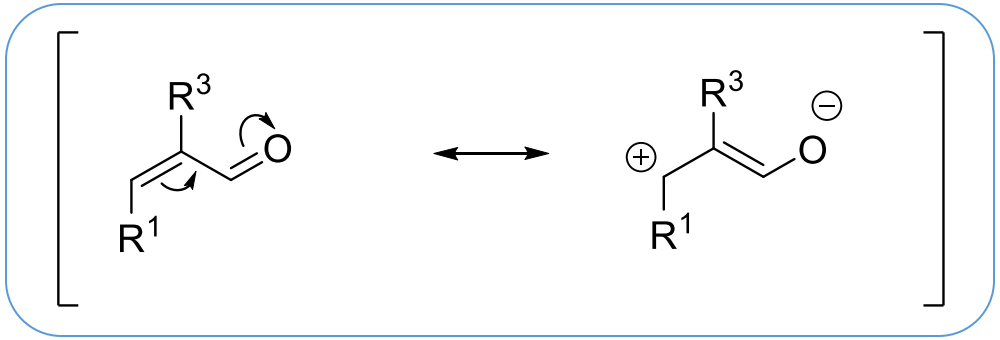
SYNTHESIS

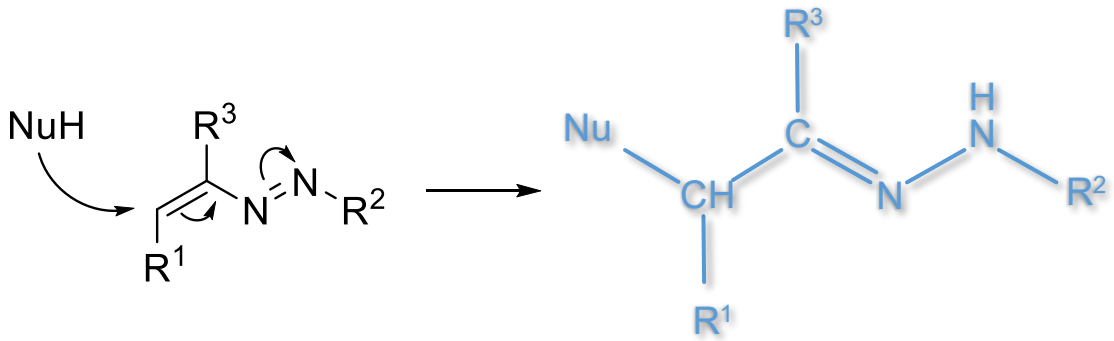




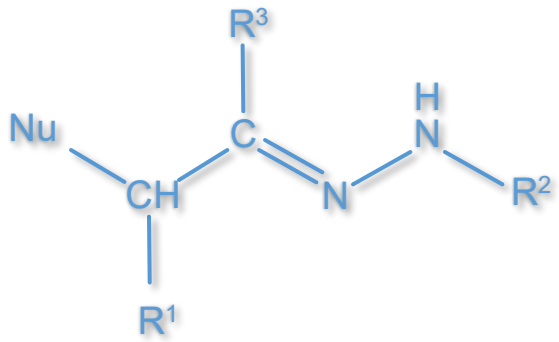
REACTIVITY

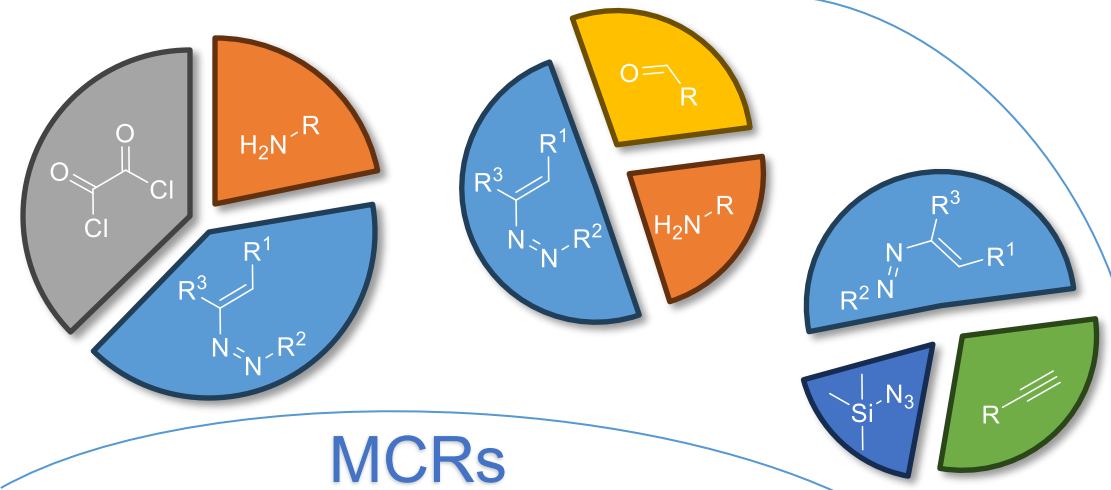






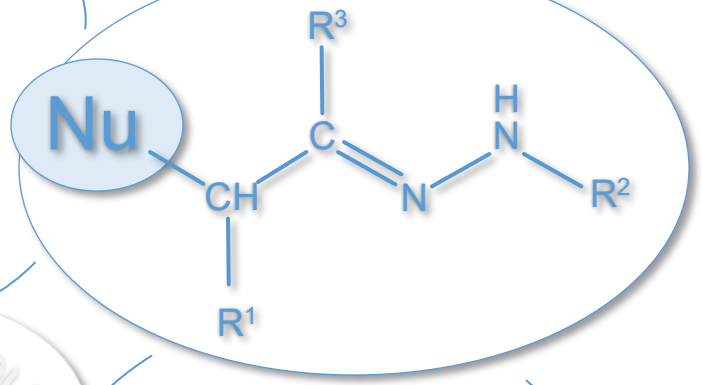
Michael 1,4 addition

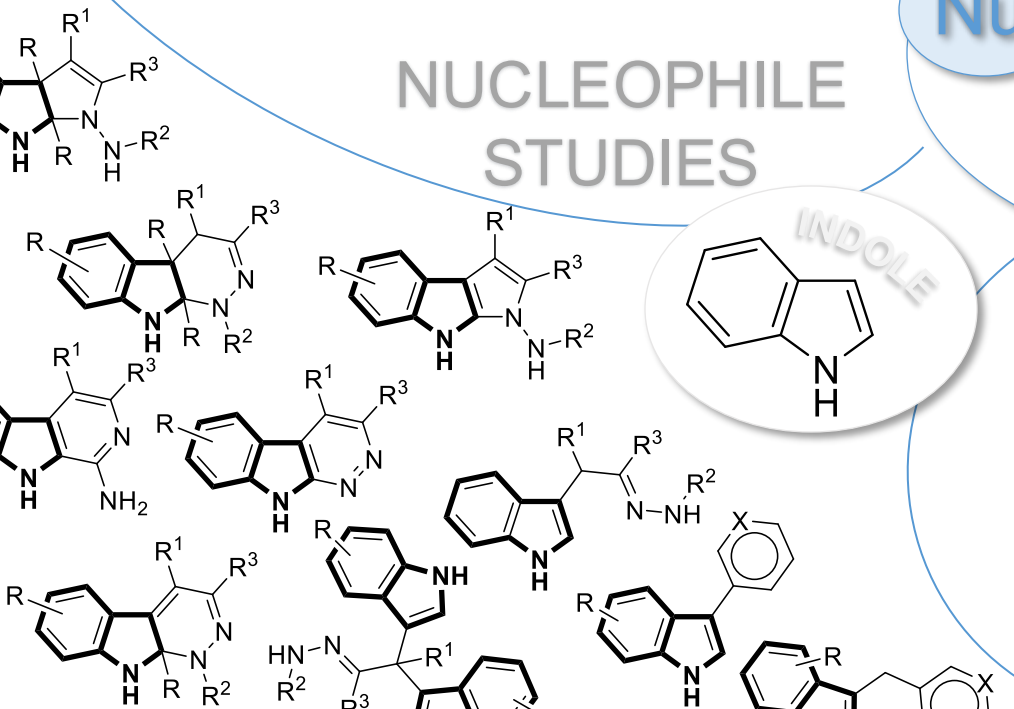

R3
Nu
C
H
N
CH
N
R2
R1

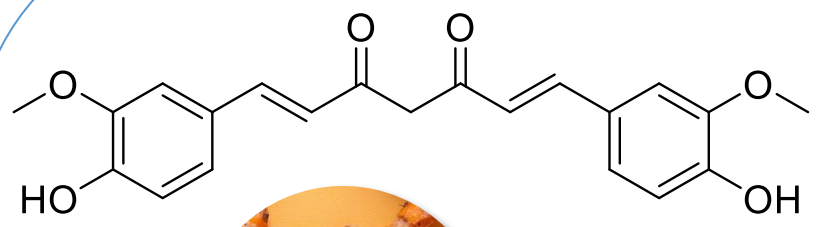


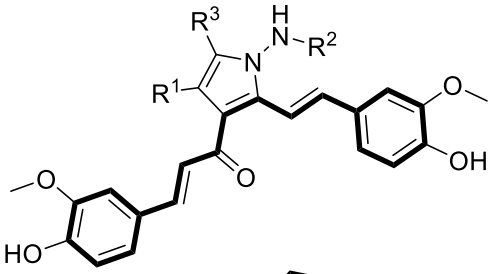
MCRs DEVELOPMENT

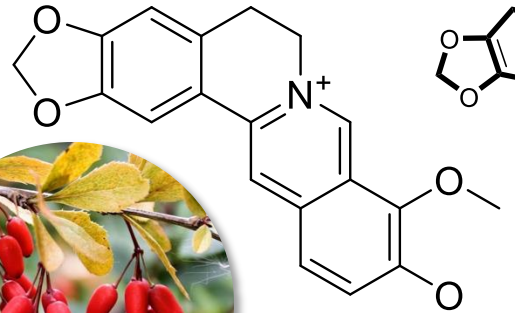
NUCLEOPHILE STUDIES

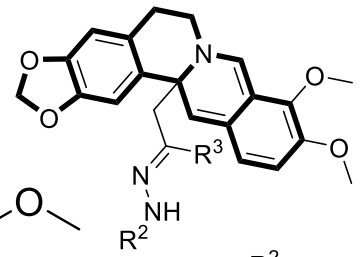


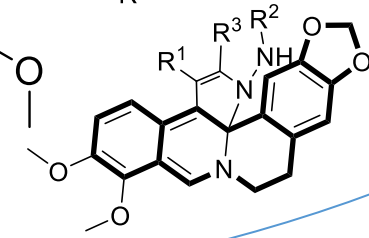






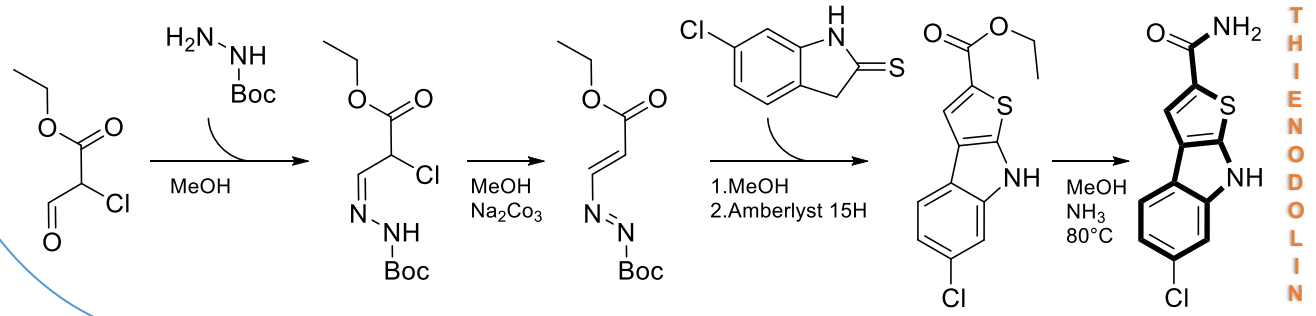






NATURAL COMPOUNDS

TOTAL SYNTHESIS

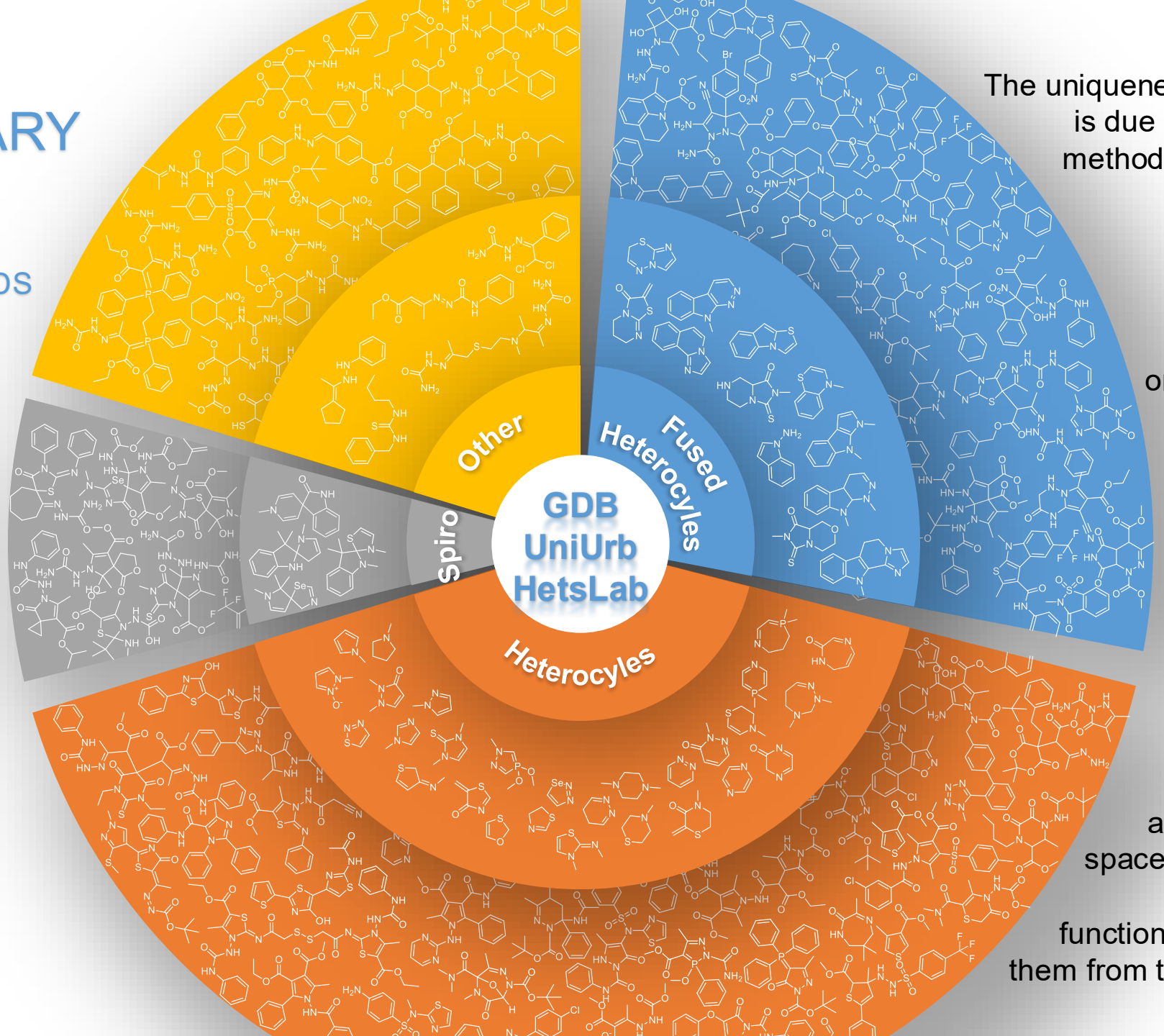


UNIURB PROPRIETARY LIBRARY

MORE THAN 2500 UNIQUE COMPOUNDS

The idea is that local libraries display more *diversity*, *uniqueness*, and chemical *complexity* with respect to standard commercial libraries.

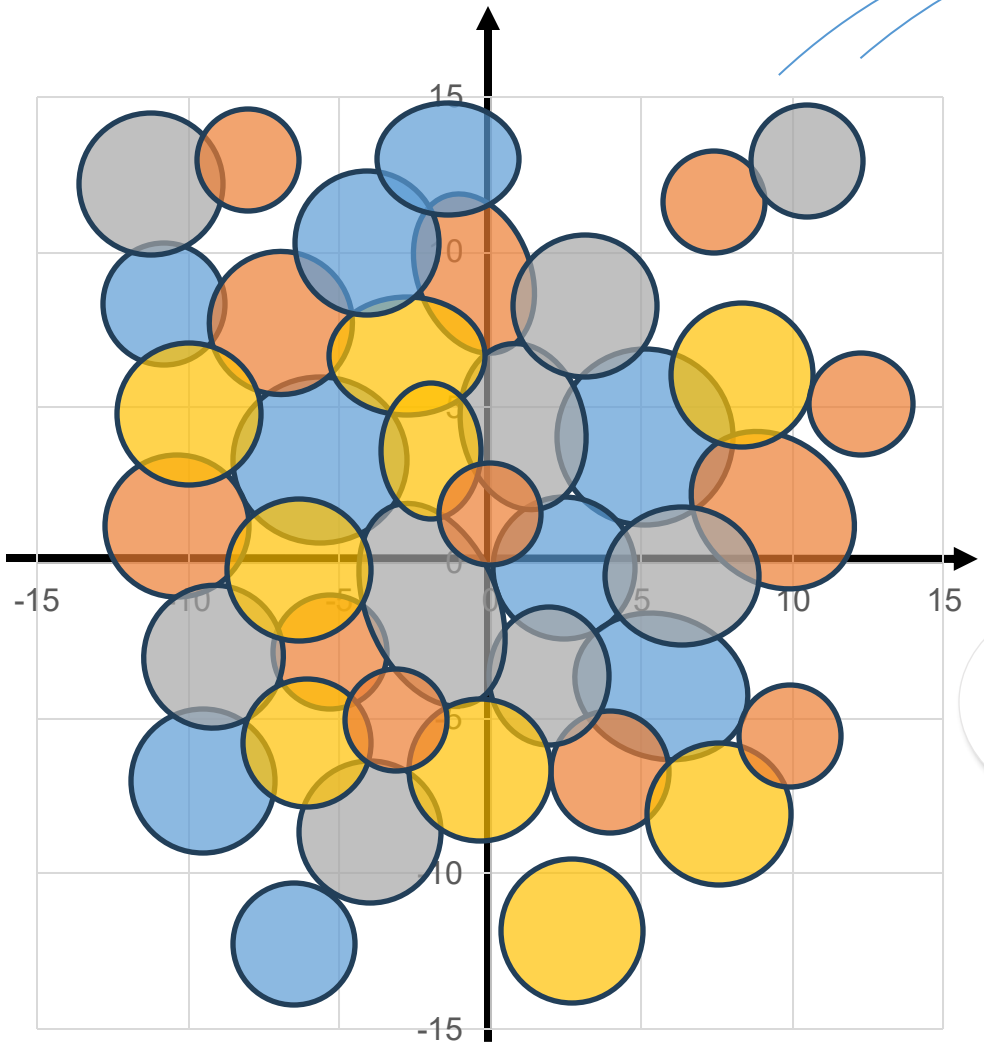
This activity will likely enhance
a) the chance to generate IP thanks to the computational platform
b) the attractiveness of the platform for external users.



The uniqueness of the Uniurb library is due to the unique synthesis methods developed by several teams over the years. These original and innovative approaches have made it possible to synthesize not only privileged scaffolds, which are already difficult to synthesize in a convenient way, but to functionalize them with extreme simplicity, giving rise to a series of new compounds. The essential characteristic of these derivatives is that they are placed in a chemical space that is still unexplored; the richness of their functionalizations differentiates them from those already available.

1st VIRTUAL SCREENING

BASED ON CHEMICAL DIVERSITY

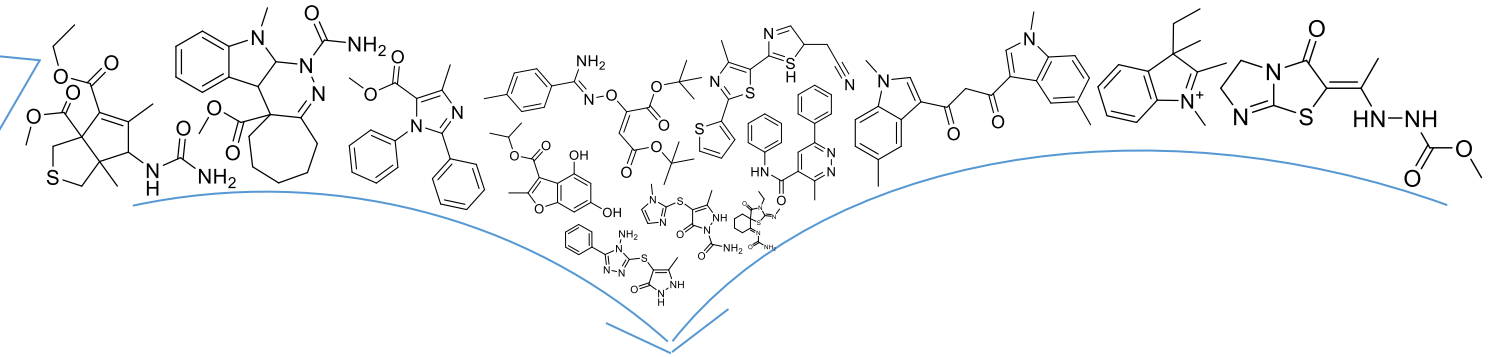


CLUSTERS CREATION

CLUSTER SCREENNIG

UNDER SCREENING

37 CENTROIDS AS REPRESENTATIVE COMPOUND OF EACH CLUSTER



IN VITRO SCREENING

Prof. Galluzzi
ANTILEISHMANIAL

2 LEAD FOUNDED

Prof.ssa Frangipani
ANTIBCATERIAL ACTVITY
Staphylococcus aureus

2 LEAD FOUNDED

Prof. Brandi
Prof. De Santi
ANTITUMORAL STUDIES
2D and 3D cancer cells (MDA-MB-231)

3 LEAD FOUNDED

Prof.ssa Crinelli
ANTITUMORAL STUDIES
Deubiquitinase USP2 inhibitor

UNDER SCREENING

FIRST PUBLICATION

ROYAL SOCIETY OF CHEMISTRY

View PDF Version | Previous Article | Next Article

Check for updates

DOI: 10.1039/D4RA02790F (Paper) *RSC Adv.*, 2024, **14**, 15713-15720

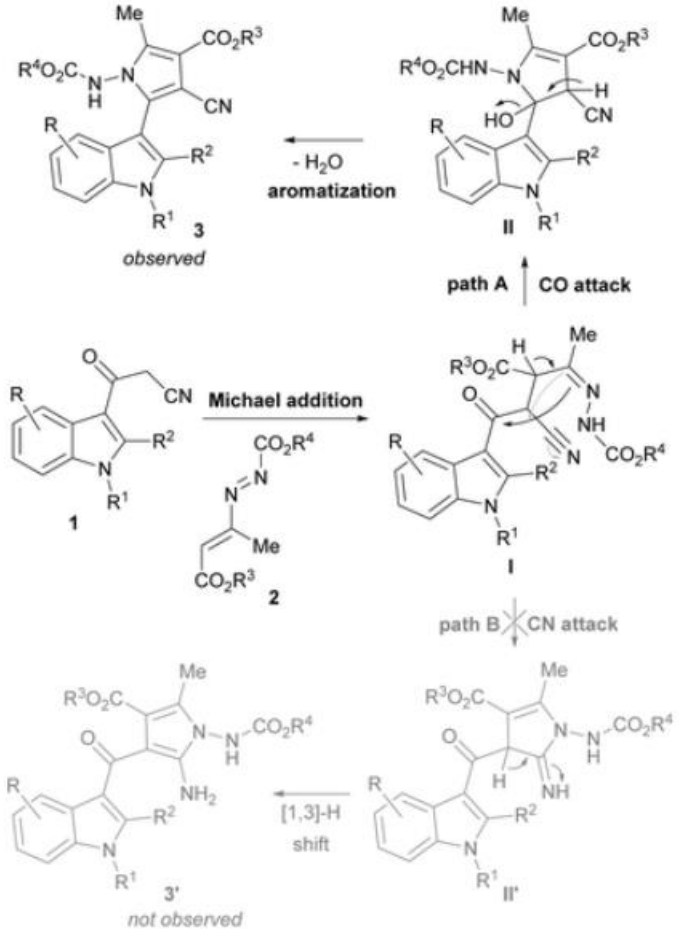
Easy one-pot synthesis of multifunctionalized indole–pyrrole hybrids as a new class of antileishmanial agents†

Vittorio Ciccone‡, Aurora Diotallevi‡, Miriam Gómez-Benmansour, Sara Maestrini, Fabio Mantellini, Giacomo Mari, Luca Galluzzi, Simone Lucarini * and Gianfranco Favi *

Department of Biomolecular Sciences, University of Urbino Carlo Bo, 61029 Urbino (PU), Italy. E-mail: simone.lucarini@uniurb.it; gianfranco.favi@uniurb.it; Tel: +39-0722303333 Tel: +39-0722303444

Received 15th April 2024 , Accepted 7th May 2024

First published on 14th May 2024



Finanziato dall'Unione europea
NextGenerationEU

Ministero dell'Università e della Ricerca

Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

UniUrb_Hetslab: a unique virtual library for computational hit identification

Università degli Studi di Urbino
23 maggio 2024

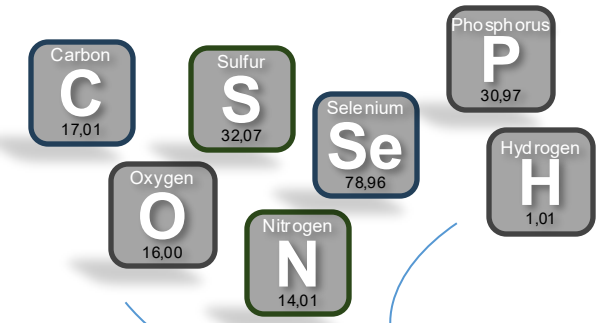
MANY THANKS

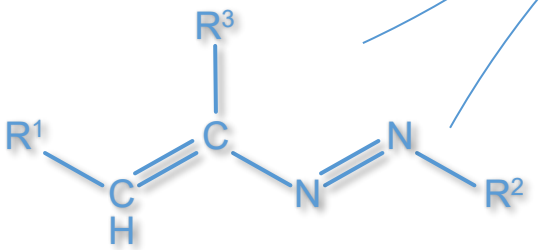
VITALITY

UNIURB PROPRIETARY LIBRARY

MORE THAN **2500** COMPOUNDS

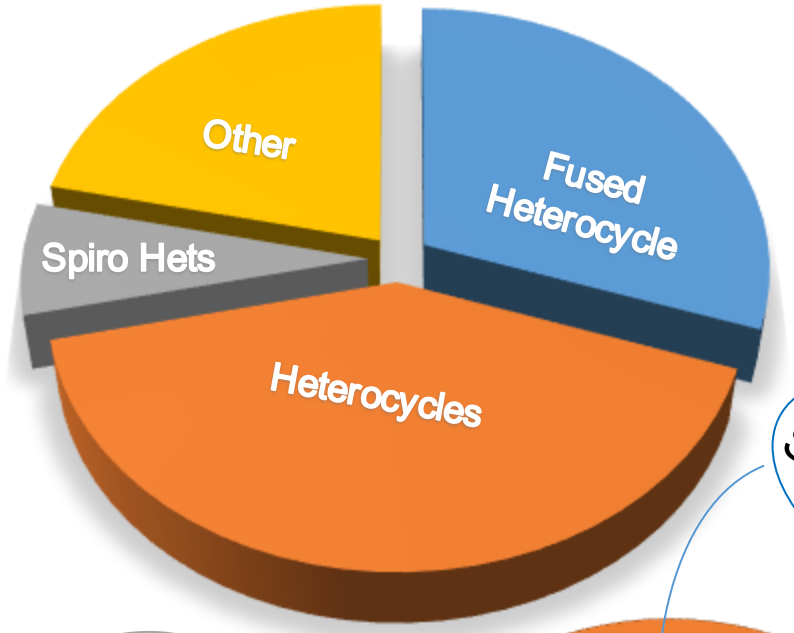
GDB-UniUrb-HetsLab



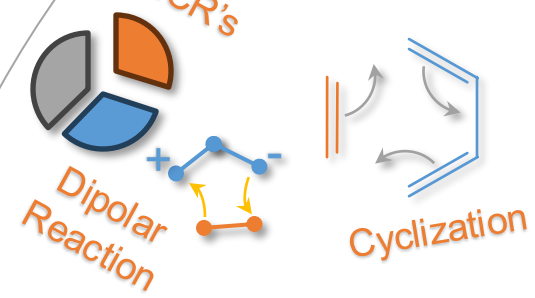


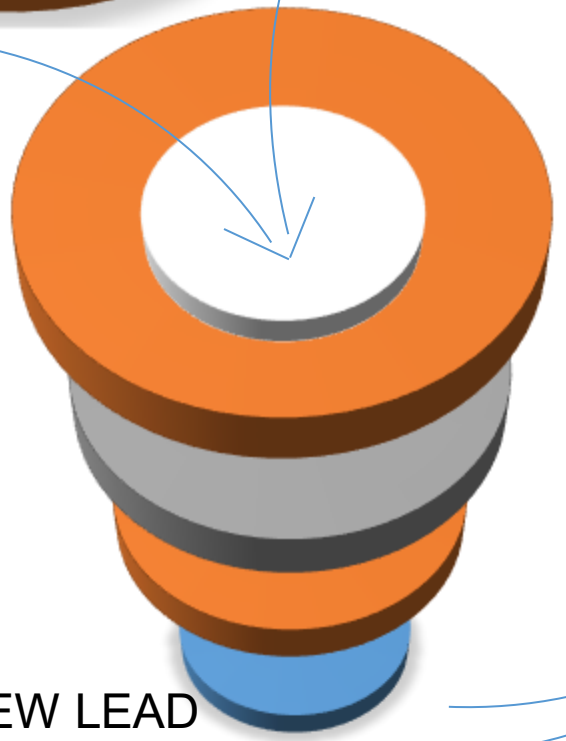
UNIQUE BUILDING BLOCK

This activity aims at compiling a virtual library of novel compounds synthesized at UNIURB over the years, which are: available or that b) can be readily synthesized thanks to the proprietary expertise at UNIURB



NEW SYNTHESIS METHODS

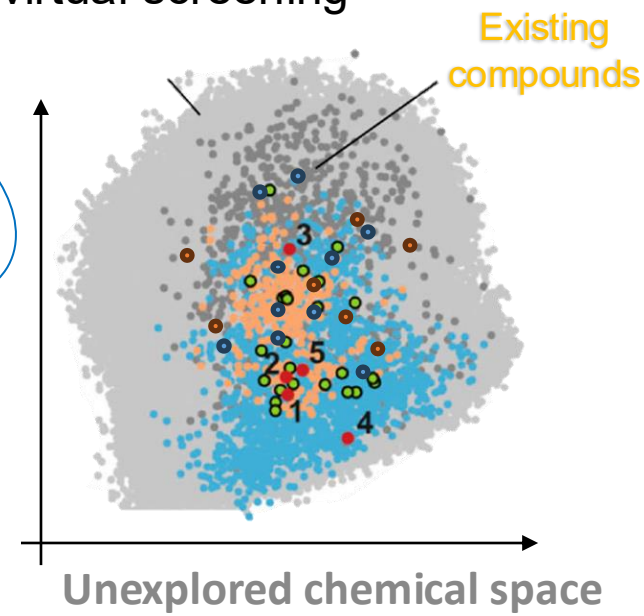




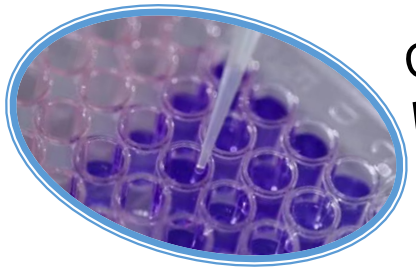
NEW LEAD GENERATION

VIRTUAL SCREENING

Assess the chemical diversity of the assembled library within the framework of commercial libraries and test it in other **Task 1** activities involving virtual screening



Identify a suitable diversity subset to be tested in targets and/or cell lines relevant to the project.



CELL LINES ASSAYS

DOI: 10.1039/D4RA02790F (Paper) *RSC Adv.*, 2024, **14**, 15713-15720

Easy one-pot synthesis of multifunctionalized indole–pyrrole hybrids as a new class of antileishmanial agents†