LIGHT-RING

Light-Driven Functionalization of Unreactive Sites Using Oxidative Amination

doc. dr. sc. Davor Šakić

HRZZ
Croatian Science Foundation

LIGHT-N-RING

Light-Driven Functionalization of Unreactive Sites Using Oxidative Animation
LIGHT-N-RING

Funded by:

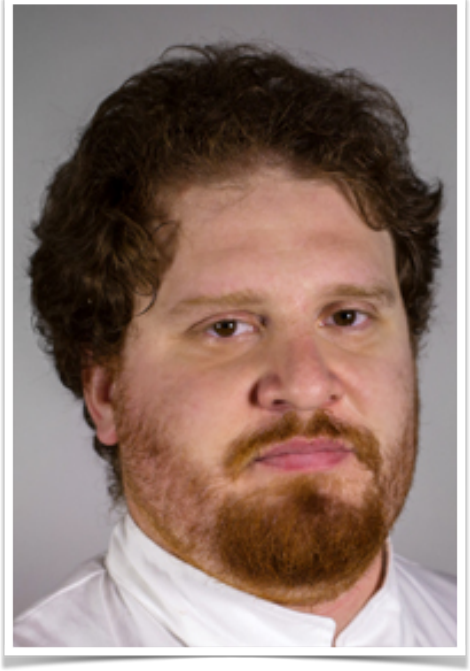
HRZZ
Croatian Science Foundation

Supported by:

Project details

doc. dr. sc. Davor Šakić
HRZZ project UIP-2020-02-4857
February 1, 2021 – January 31, 2026
Project budget: 2 000 000,00 kn
Location: University of Zagreb,
Faculty of Pharmacy and Biochemistry

Team



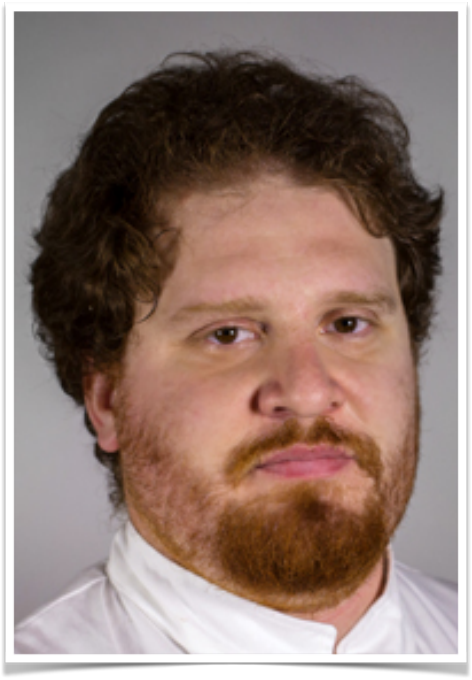
doc. dr. sc. Davor Šakić

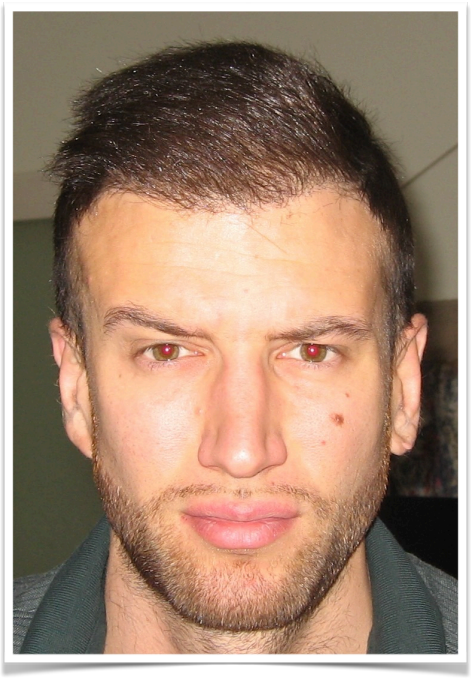
dr. sc. Mirsada Ćehić

dr. sc. Ana Karković Marković

Team

Gabrijel Zubčić, mag. appl. chem.



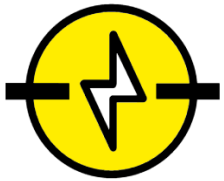


dr. sc. Ana Karković Marković

dr. sc. Mirsada Ćehić

doc. dr. sc. Davor Šakić

Collaboration



Prof. Hendrik Zipse, Ludwig-Maximilian University, Munich, Germany

mixed computational and organic synthesis lab with ample experience in radical chemistry and advanced organic synthesis

Prof. Armin R. Ofial, Ludwig-Maximilian University, Munich, Germany

extensive experience in stopped-flow and quench-flow techniques

Prof. Moisés Canle López, University of A Coruña, A Coruña, Spain

expertise in laser-flash photolysis and radical trapping

Research

Facilities:

University of Zagreb, Faculty of Pharmacy and Biochemistry (pharma.unizg.hr)

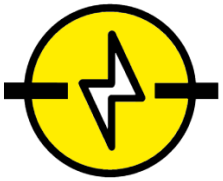
FarmInova lab @ Center for Translational Research and Innovation in Pharmacy

thermodynamic lab @ Department of General and inorganic Chemistry

kinetics lab @ Department of Physical Chemistry

NMR lab @ Department of Organic Chemistry

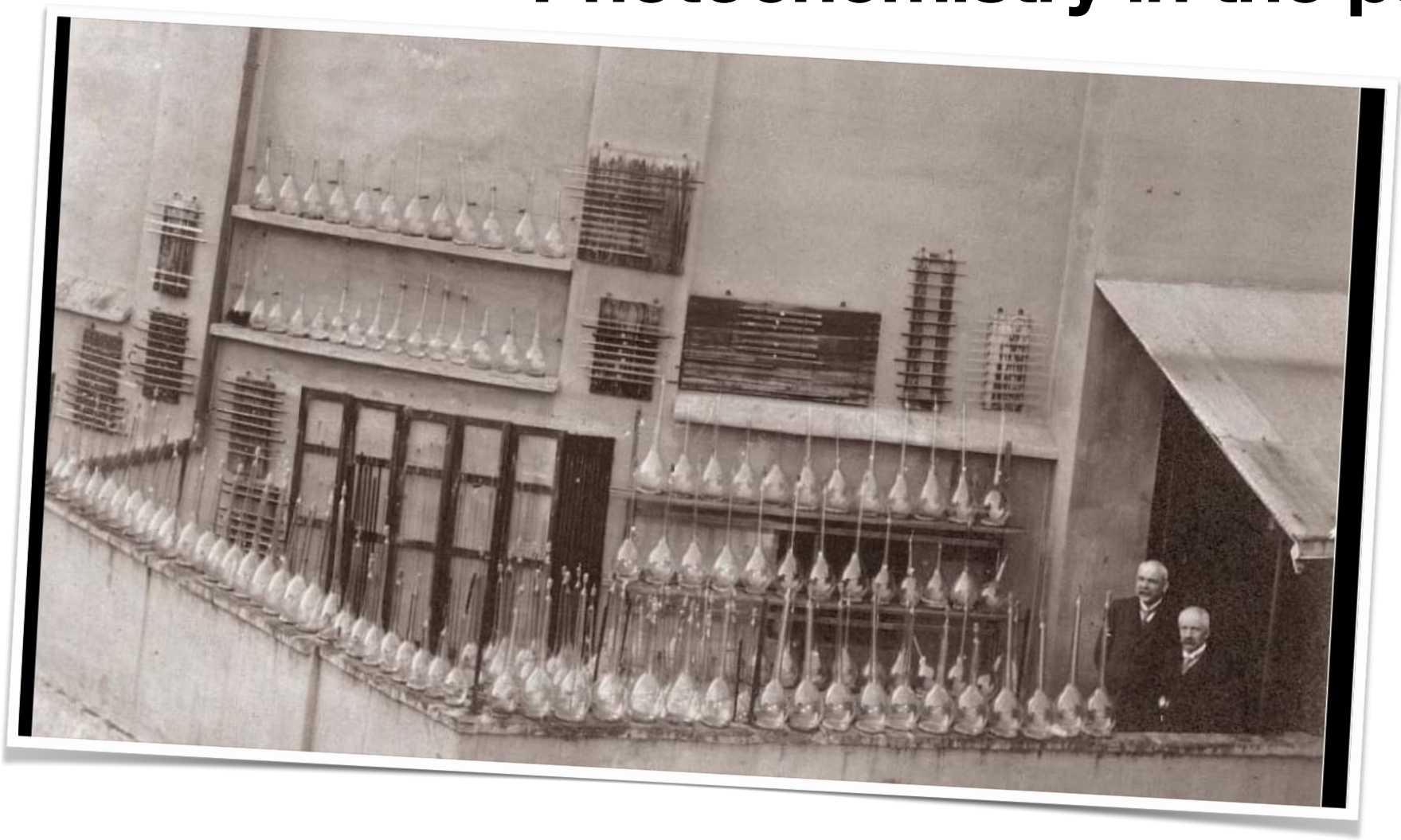
EPR lab @ Department of Biophysics



University of Zagreb, University Computing Centre (SRCE)

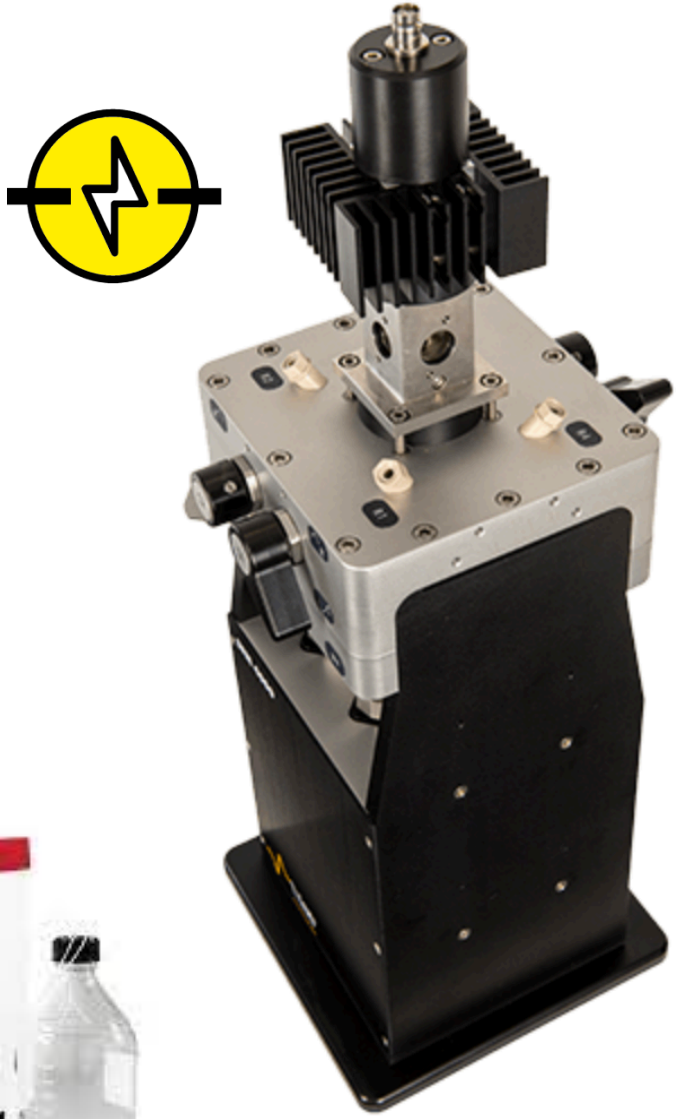
Isabella Cluster @ SRCE (https://www.srce.unizg.hr/en/isabella-cluster)

Photochemistry in the past



Research

Equipment:

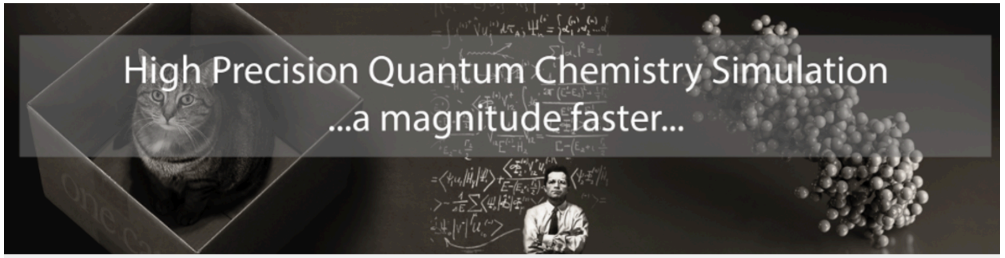


Research

Programs & workstations:

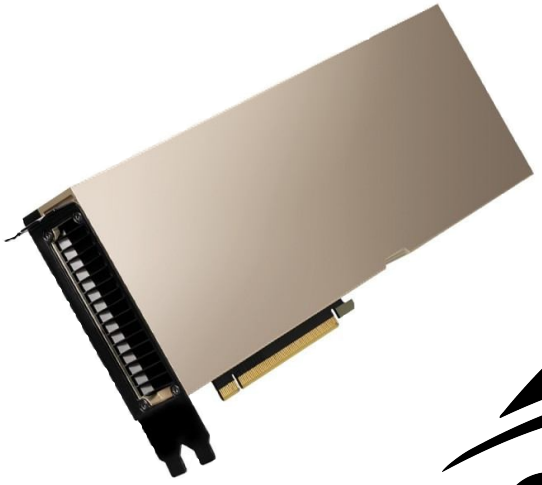
PetaChem

Chemistry at the speed of graphics...



GPU module for Q-CHEM: BrianQC

BrianQC is a GPU module for Q-Chem. It speeds up Density Functional Theory and Hartree-Fock single point, geometry optimization and frequency calculations and many other methods.
Additionally use BrianQC as a quantum chemical Software Development Kit (SDK) and build the application you want.



ORCA

Q-CHEM™

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Publications

Organic & Biomolecular Chemistry

PAPER

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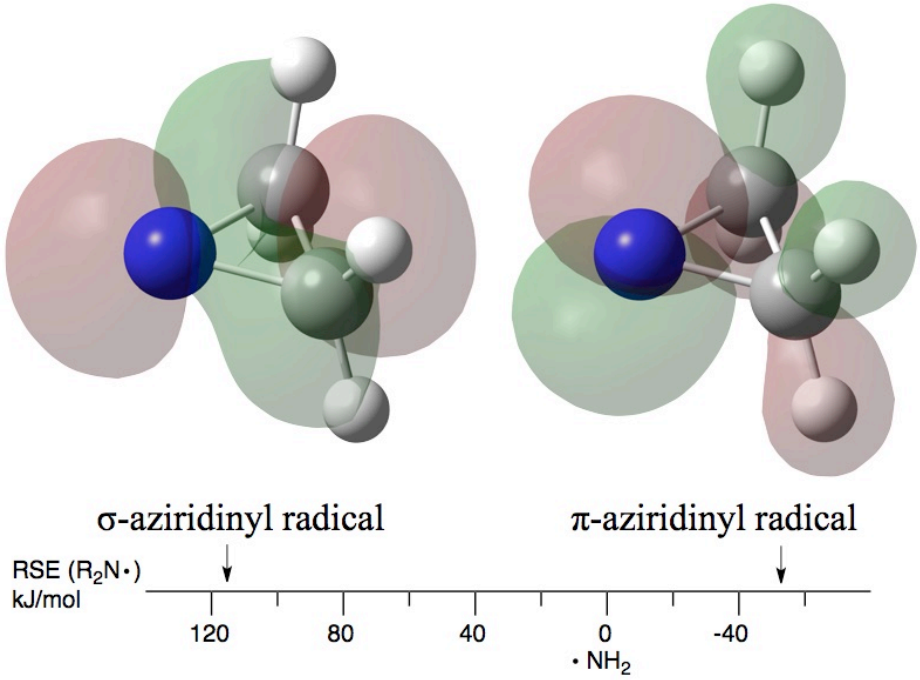
The stability of nitrogen-centered radicals†

Johnny Hioe,[a] Davor Šakić,[b] Valerije Vrček*[b] and Hendrik Zipse*[a]

Cite this: *Org. Biomol. Chem.*, 2015, **13**, 157



Publications

FULL PAPERS DOI: 10.1002/adsc.201600629

Advanced Synthesis & Catalysis

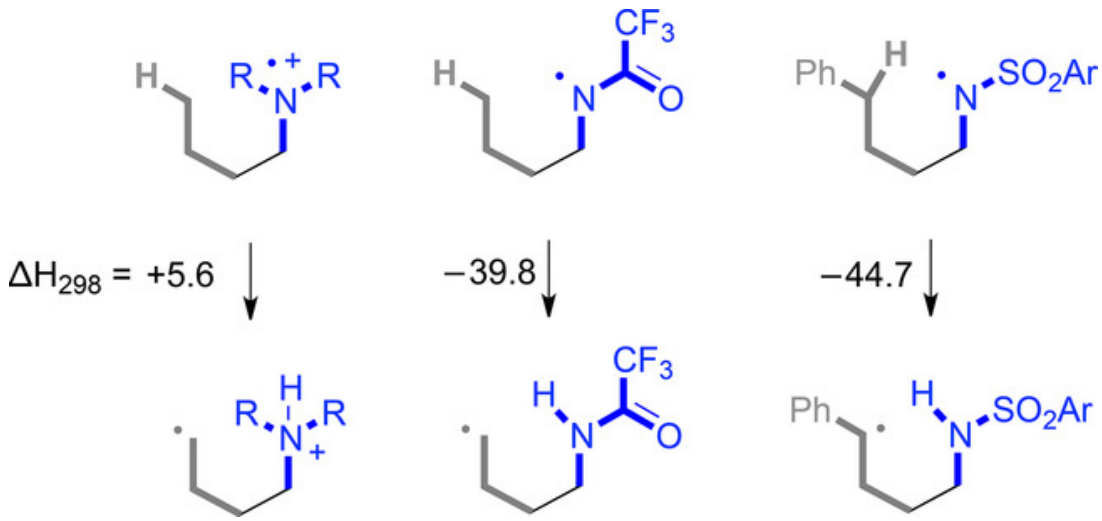
Very Important Publication

Radical Stability as a Guideline in C–H Amination Reactions

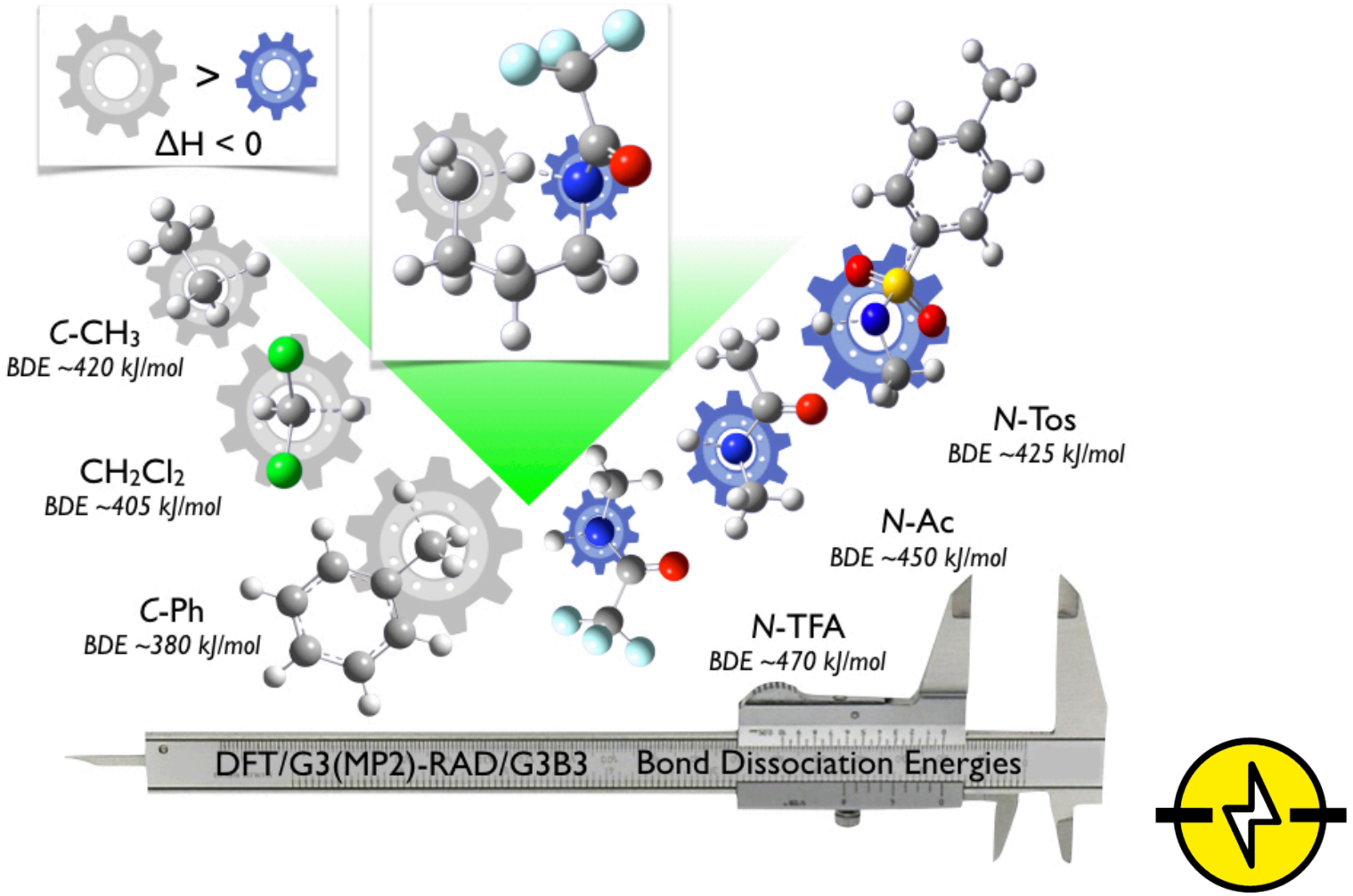
Davor Šakić[a] and Hendrik Zipse[b,*]

[a] University of Zagreb, Faculty of Pharmacy and Biochemistry, Ante Kovačića 1, 10000 Zagreb, Croatia
[b] Department of Chemistry, LMU Muenchen, Butenandtstrasse 5–13, 81377 Muenchen, Germany
Fax: (+49)-89-2180-77738; phone: (+49)-89-2180-77737; e-mail: zipse@cup.uni-muenchen.de

Received: June 17, 2016; Revised: August 22, 2016; Published online: September 21, 2016



Publications



Publications

Organic & Biomolecular Chemistry

ROYAL SOCIETY OF CHEMISTRY

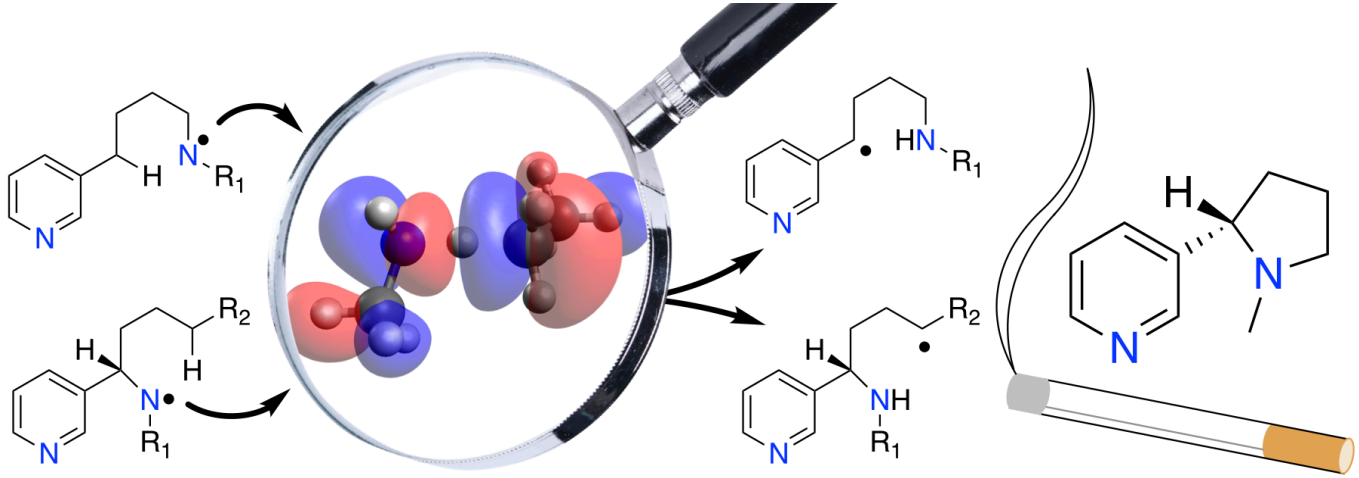
PAPER

Check for updates

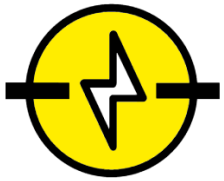
Cite this: *Org. Biomol. Chem.*, 2021, **19**, 854

Role of substituents in the Hofmann–Löffler–Freytag reaction. A quantum-chemical case study on nicotine synthesis†‡

Sofia Shkunnikova,[a] Hendrik Zipse [b] and Davor Šakić *[a]

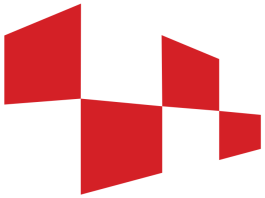


Activities



- Establishment of the new research group
- Computational modelling of the HLF reaction mechanism and parameters of its regiospecificity
- Quantifying the role of the oxidant in the shift from inter- to intramolecular HAT steps
- Fine-tuning of the N-centered radicals' stability in order to increase the number of available substrates. EPR investigation of radical generation by irradiation or electrochemically.
- Finding a switch between radical and ionic pathways, which can be utilized to develop stereospecific transformations, or activate unreactive substrates
- Preparation of a new research proposal: Application of the HLF procedure in pharmaceutical synthesis

Thank you



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