Plan Overview

A Data Management Plan created using DMPTool

Title: Light-Driven Functionalization of Unreactive Sites Using Oxidative Amination, LIGHT-N-RING

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Template: Digital Curation Centre

Project abstract:

In this project, the mechanism of metal-free C-H bond amination reactions will be explored to discover necessary chemical switches and/or reaction conditions to further increase the chemo-, regio-, stereo-specificity and the utility of these reactions. The goal is to quantify the effects of various electron-withdrawing groups on the N-centered radical (in)stability, which directly relates to the driving force of the reaction and uses this data for the rational design of HLF reactions. Competition between intra- and inter-molecular pathways must be analysed in more detail in order to offer a better understanding of the regioselectivity of the reaction. The underlying reaction mechanism needs a detailed re-evaluation after demonstrating that some reaction variants proceed through ionic mechanisms to products with intact stereochemical information. A detailed search for a chemical switch that governs which mechanism is active in selected reactions will be conducted.

Start date: 02-01-2021

End date: 01-31-2026

Last modified: 01-29-2022

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

Quantum-chemical data (coordinates .xyz, energies and frequencies .g98.out, surfaces .cube)

MS, NMR EPR spectra (.jdx, JCAMP-DX, .pdf)

UV/Vis, Fluorescence, Raman and IR spectra (tables, .pdf, .jdx)

- present databases include https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi, https://webbook.nist.gov/chemistry/, https://atct.anl.gov; use of styles provided here

Coordinates will be saved in .xyz and .sdf format.
Naming convention folder: PROJECT -> WORK PACKAGE -> FAMILY (of compounds) -> COMPOUND
Naming convention subfolders: QC, UV/Vis, NMR, EPR, MS, IR
Naming convention files: COMPOUND_METHOD_CONFORMER_VERSION

Final manuscript (before submission to publication);
Authors and affiliation;
Bibliography;
Short description of data stored in repository, methods and procedures;
Description on conventions used to generate data;
Guide to relevant data;
Versioning;
Licence

JDX viewer

HTML5 viewer with JSmol/3Dmol.js

No ethical issues will arise, due to not using biological samples, and not using compounds in further biological testing.

Data is owned by authors, by institution of employment (University of Zagreb Faculty of Pharmacy and Biochemistry), and funding institution (Croatian Science Foundation).
There are no restrictions to reusing of data.
Sharing of full data will be postponed till scientific article is published.

Chosen licence is:

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- **No additional restrictions** — The end user may not apply legal terms or technological measures that legally restrict others from doing anything the license permits.

Local storage during project year. Periodic publication on the projects' web-page (https://sw.pharma.hr/light-n-ring/).

Free of charge digital repositories: https://dabar.srce.hr and https://zenodo.org

For programs and scripts: https://github.com

Backup of data is 90 days after project period is finished, or if manuscript is published. At least once a year.

Recovery of data will be from digital repositories.

Local data is stored on RAID-1, which consists of an exact copy (or mirror) of a set of data on two disks.

Backup of data will be once a month to a local hard drive, connected to the cluster only during the backup.

Access to local data is through registered users of the research team on Cluster sw.pharma.hr.

No data is created in the field.

Access and security of digital repositories is the sole responsibility of used digital repositories.

Coordinates of all calculated species needed to recreate/recalculate published results. Formats used: .xyz, .sdf, .mol. Searchable through SMILES and chemical formula. - long term storage

Formatted checkpoint files with electron distribution. - short term storage

Spectra in .csv and .jdx data format. - long term storage (digital repositories) https://cenapt.pharm.uic.edu/tutorials/NMRdataSharing_DATAVERSE_Protocol-6.pdf

Usage of free long-term repositories. Time for preparing data for sharing and preservation is allocated during the course of the project.

Data will be first available through supporting information (SI) file accompanying published article. This SI file will have reference and path to the digital repositories where additional data is to be stored. SI files are provided free of charge at journals' publisher website. Data is shared with CC BY 4.0 licence. Direct request will be pointed to the respective digital repositories. Full data will be available as soon as the article is accepted. It will be associated with DOI of the scientific article and additionally by url and digital identifier number from the digital

repositories.
Reuse of data is permitted under CC BY 4.0 licence, with references to the authors of the involved data.

In this project data has exclusive use only until it is shared via publication in scientific journal. No data sharing agreement will be needed.

Project leader, assis. prof. Davor Šakić is responsible for implementing this DMP. He will review and revise this plan every year until project end.
Data management activity will be shared by projects' members. During collaboration, all data will be jointly shared.

Roles:
Data capture - all project members
Metadata production - all project members, revised by project leader
Data quality assessment - project leader
Local storage and backup - administrator of the cluster and/or project leader
Data archiving - project leader
Data sharing - all project members

Free online training will be found for expertise in data management. Specialists of the http://dabar.srce.hr repository will be contacted for additional support and potential troubleshooting.
Additional hardware is planned in the budget (additional backup storage capacity in RAID-1 configuration).

Planned Research Outputs

Dataset - "Reactions of nitrogen centered radicals "

Geometries and calculated energies of reaction pathways for rearrangement on N-centered radicals. Kinetic UV/Vis, NMR, HRMS, and EPR spectra.

Planned research output details

Title	Type	Anticipated release date	Initial access level	Intended repository(ies)	Anticipated file size	License	Metadata standard(s)	May contain sensitive data?	May contain PII?
Reactions of nitrogen centered radicals	Dataset	2023-01-31	Open	GitHub Zenodo DABAR	2 GB	Creative Commons Attribution 4.0 International	None specified	Yes	No