ELECTROCATALYTIC DEHYDROGENATIVE COUPLING OF OLEFINS TO DIENES

A Data Management Plan created using DMPonline.be

Creator: Harry Poels-Ryckeboer

Affiliation: KU Leuven (KUL)

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Template: FWO DMP (Flemish Standard DMP)

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Project abstract:
Conjugated dienes, and in particular 1,3-butadiene, are essential molecules in chemistry, e.g. for
rubber production. Current synthesis routes face limitations, e.g. because of changing feedstocks or
high energy demand. We here propose to couple olefins like ethylene directly to one another, with
net removal of 2 H-atoms. The proposal is based on the applicant's finding that Pd, in combination
with a hydroxypyridine ligand, can couple olefins to dienes with oxygen scavenging the hydrogen
atoms. In order to avoid risks and side reactions linked to oxidants, we now propose to funnel away
electrons from the Pd catalyst to an anode, while the protons are cathodically reduced to H_2. In this
translation of a homogeneous catalytic reaction to an anodic process, electrode choice, ligand and
mediator selection and electroreactor design are key elements. Mechanisms are investigated by
combining cyclic voltammetry with spectroscopy (e.g. XAS). Thorough attention is given to
reactivating the catalyst, especially if the zerovalent Pd aggregates to large particles; chemical
treatments as well as electrochemical procedures are investigated to restore the activity. Since future
ethylene might be produced by electroreduction of CO_2, we also examine whether the ethene-tobutadiene reaction would be sensitive to
by-products of the CO_2 reduction, like CO. Finally, the
reaction's scope is expanded to produce fine chemicals like medicines and fragrances by crosscoupling.

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1. Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset Name	Description	New or reused	Digital or Physical	Only for digital data Digital Data Type	Only for digital data Digital Data format	Only for digital data Digital data volume (MB/GB/TB)	Only for physical data Physical volume
		Please choose from the following options: • Generate new data • Reuse existing data	*Please choose from the following options:* • Digital • Physical	*Please choose from the following options:* • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA	*Please choose from the following options:* • .por, .xml, .tab, .csv,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
GC chromatograms		new data	Digital	Experimental	.gcd	<100MB	
NMR spectra		new data	Digital	Experimental	NA	<100MB	
XAS data		new data	Digital	Experimental	.dat	<100MB	

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

NA

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

• No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

• No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, …)? If so, please comment per dataset or data type where appropriate.

- Yes

The methods and reactor configurations developed in this project have potential for valorization, which will be subjected for discussion during the project. Patents will be submitted, transferred and valorized with the assistance of the intellectual property unit of KU Leuven Research & Development (LRD).

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/Data transfer agreements/ research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

2. Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g., in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, Codebook.tsv etc. where this information is recorded).

Details to reproduce reaction procedures are described in a personal lab booklet. Upon presentation or publication of data, procedures are described in sufficient detail to enable a reproduction of the generated results for an experienced user. ReadMe-files or recording methods for advanced characterization are stored in parallel with generated data

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

- No

Although no metadata standard is available for the advanced characterization in this project, most techniques store a non-standardized ReadMe-file containing recording parameters and file information in parallel with recorded datasets. Alternatively, some datasets contain metadata headers on recording parameters. The data will be stored and named in a consistent manner with unambiguous identifiers. Descriptions of experiments and materials are kept in physical lab notes for each identifier. The data will be processed and summarized in a comprehensive excel worksheet with references to the identifiers. The resulting summaries will culminate in presentations, and finally in manuscripts and/or patents.

3. Data storage & back-up during the research project

Where will the data be stored?

Physical hand-notes of procedures and initial observations are kept in lab books. Digital data, with unambiguous identifiers for reactions and materials, are kept in cloud storage from 'Box'. KU Leuven offers an Enterprise Box account 3, which offers an easy and secure storage space of up to 100 GB for each user.

How will the data be backed up?

By using the cloud storage of 'Box', digital data will be stored in parallel on the cloud and on the personal computer of the applicant, guaranteeing back-up for this data. Most raw data is also stored and frequently backed up off-line on external hard drives.

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely. If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.

- Yes

The cloud storage provides a storage space up to 100 GB for each user, while the project is expected to generate less than 10 GB.

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

The data will be stored in the university's secure environment for private data. An Enterprise Box account 3 for cloud storage ensures a secure environment.

What are the expected costs for data storage and backup during the research project? How will these costs be covered?

Data storage costs on Box are included in an internal service contract with the KU Leuven IT support service (SET-IT). No additional costs are expected for the storage of data. In case additional costs do arise, they will be covered by the project budget or reserve funds.

4. Data preservation after the end of the research project

Which data will be retained for at least five years (or longer, in agreement with other retention policies that are applicable) after the end of the project? In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).

All data will be retained for the expected 5 year period after the end of the project.

Where will these data be archived (stored and curated for the long-term)?

Upon termination of the contract, the data will be transferred and stored on an external hard drive (Samsung Portable SSD T5 1 TB), managed by Annelies Van Vlasselaer.

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4 of 6

What are the expected costs for data preservation during the expected retention period? How will these costs be covered?

The high capacity of the available external hard drive (1 TB) enables the preservation of data from multiple terminated or finished projects. Currently, an average of 15 GB is used for the finished projects of each user, which allows to divide its cost over approximately 60 users. Given the cost of the available hard drive of 120 EUR, the expected costs are negligible. The involved IT-expenses are included in the project's consumable expenses or covered by reserve funds.

5. Data sharing and reuse

Will the data (or part of the data) be made available for reuse after/during the project? In the comment section please explain per dataset or data type which data will be made available.

- Yes, in a restricted access repository (after approval, institutional access only, …)

If access is restricted, please specify who will be able to access the data and under what conditions.

Only uses for research purposes will be allowed and commercial reuse will be excluded.

Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)? Please explain in the comment section per dataset or data type where appropriate.

- No

Where will the data be made available? If already known, please provide a repository per dataset or data type.

Upon request by mail

When will the data be made available?

Upon publication of the research results

Which data usage licenses are you going to provide? If none, please explain why.

None, not applicable.

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- Yes

DOI corresponding to the DOI of the publication.

What are the expected costs for data sharing? How will these costs be covered?

No additional costs are expected as the data can be shared via online platforms (e.g. WeTransfer) or the already budgeted storage cloud from Box. If additional costs would occur they
will be covered from reserve funds.

6. Responsibilities

Who will manage data documentation and metadata during the research project?

The applicant (Harry Poels-Ryckeboer)

Who will manage data storage and backup during the research project?

The applicant (Harry Poels-Ryckeboer)

Who will manage data preservation and sharing?

The applicant (Harry Poels-Ryckeboer)

Who will update and implement this DMP?

The applicant (Harry Poels-Ryckeboer)