



Newsletter No.2 October 2022

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A research project funded under the EU H2020 programme, developing enzymes for environmental-friendly products

Welcome from the OXIPRO Project Coordinator, Dr. Gro Bjerga

Welcome to our 2nd Newsletter

We're happy to announce that OXIPRO is now fully operationalised, and our first outcomes have been achieved.

We have published three original OXIPRO papers based on work across partnerships in the project, and also joint initiatives with our sister projects. We have also contributed to a number of conferences and meetings with scientific advancements and policy input.



We invite you to collaborate with us, to create change and to shape OXIPRO's developments and the future of enzyme applications. Please [register via our website](#) to stay up to date with our initiative and to take part in our events. For 2023 we will be organising several events around topics of enzyme technologies for more environment-friendly consumer products in the context of a circular economy. We welcome your participation. If you want to know how we engage those interested in OXIPRO, we've taken a "scientific approach" and [published our guide](#) on how to develop a stakeholder engagement plan.

Meet our partners - LEITAT

OXIPRO Biotech Team at LEITAT

LEITAT's expertise lies in R&D, technology transfer and industrial innovation services. Meet the OXIPRO biotech team (from left to right in the photo): Belen Castro, Helena Balfagon, Arnau Bassegoda and Aroa Rey Campa. Belen and Helena have recently joined the team, and are junior researchers involved in the technical aspects of WP4 and WP5. Arnau coordinates the cosmetics case study and Aroa leads WP5, coordinates the detergent case study and is a member of the scientific committee.



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Updates from our consortium

OXIPRO's first face-to-face meeting

Since you last heard from us, team OXIPRO gathered together for a long-awaited face-to-face gathering in Groningen, Netherlands for the annual project meeting. The event enabled OXIPRO partners to share research highlights and plan ongoing interactions and collaborations. We were delighted to be joined by counterparts from our sister project [FuturEnzymes](#).



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NORCE at Bioflavour Conference

Delegates from OXIPRO's coordinating partner organisation NORCE recently participated in the Bioflavour Conference, held this year from 27th – 30th of September in Frankfurt, Germany.

Over 150 participants from more than 17 countries represented different industries, research institutes and universities at the conference, which was organised to bring recent biotechnological developments in the synthesis and production of flavour, fragrance, and functional compounds.

Dr Gro Bjerga, our Project Coordinator, delivered a flash presentation about our work.

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RUG representation at the Netherlands Biotech Congress

OXIPRO partner [Marco Fraaije \(RUG\)](#) recently took part in the [Netherlands Biotechnology Congress](#), held on 4 October 2022 at the Corpus Congress Centre in Leiden. In a full programme of keynotes, plenaries and parallel sessions, Marco chaired a session on food, which looked at biotech solutions currently underway to address global challenges, among other research foci. The programme and abstracts are available [here](#).

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Rolco features at 2nd Sustainable Homecare Products Forum

OXIPRO partner Rolco, represented by Research and Development Director, Panos Kotsakis, recently showcased OXIPRO's work in a presentation titled: "Future outlook on the HomeCare industry: Sustainable product development" at the 2nd Annual Sustainable HomeCare Products Forum, Frankfurt, Germany. The talk focused on issues surrounding weight efficient sustainable raw materials; packaging; product compaction; and consumer habit change

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From Spain to Turkey on a cotton fact-finding mission

OXIPRO partners Óscar Romero and Yerko Fredes, researchers from the Department of Chemical, Biological and Environmental Engineering of Universitat Autònoma de Barcelona (Spain) have made a fruitful visit to the facilities of the Zorluteks (Turkey). Gizem Aydemir, textile engineer in charge of Zorluteks' participation in OXIPRO, guided them around Zorluteks, showing all the steps of the cotton treatment process. Marina Guillen Montalban (Senior Researcher, UAB) commented, 'This was a great opportunity to discover more about each step of the cotton treatment process'.

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First scientific paper published

OXIPRO partners are proud to announce their first scientific publication. Titled “Structural Elucidation and Engineering of a Bacterial Carbohydrate Oxidase”, it is the result of the ongoing fruitful collaboration between the University of Groningen (RUG), led by Marco Fraaije, and Barcelona Supercomputing Center (BSC), led by Victor Guallar. Two young stars of the teams, Lars Santema (RUG) and Ruite Xiang (BSC), also significantly contributed. Focusing on a carbohydrate oxidase, the paper is of relevance to OXIPRO’s innovation cases and [downloadable here](#)

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Partners publish a fail-safe 10-point plan for stakeholder engagement

OXIPRO partners [SB Science Management](#) (SBSM) and [REDINN](#), have just published a succinct, practical guide to planning stakeholder engagement, titled ‘Ten simple rules on how to develop a stakeholder engagement plan’.

Led by Susanne Hollmann (SBSM), the paper addresses the challenges inherent in effective stakeholder engagement through a ten-point plan that provides a structured workflow.

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OXIPRO and FuturEnzyme - first joint paper by sister projects

OXIPRO is excited to announce our first joint publication with sister project FuturEnzyme. Titled ‘EP-pred: A Machine Learning Tool for Bioprospecting Promiscuous Ester Hydrolases,’ this is the result of a successful collaborative effort involving co-authors Ruite Xiang, Ana Robles-Martin and Victor Guallar from Barcelona Supercomputing Center (BSC); along with Laura Fernandez-Lopez and Manuel Ferrer, Department of Applied Biocatalysis, ICP, CSIC.

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Biochemistry
pubs.acs.org/biochemistry
Article

Structural Elucidation and Engineering of a Bacterial Carbohydrate Oxidase

Alessandro Boverio, Wahyu S. Widodo, Lars L. Santema, Henriëtte J. Rozeboom, Ruite Xiang, Victor Guallar, Andrea Mattevi, and Marco W. Fraaije*

Cite This: <https://doi.org/10.1021/acs.biochem.2c00307> | Read Online

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ABSTRACT: Flavin-dependent carbohydrate oxidases are valuable tools in biotechnological applications due to their high selectivity in the oxidation of carbohydrates. In this study, we report the biochemical and structural characterization of a recently discovered carbohydrate oxidase from the bacterium *Ralstonia solanaceum*, which is a member of the vanillyl alcohol oxidase flavoprotein family. Due to its exceptionally high activity toward N-acetyl-D-glucosamine and N-acetyl-D-glucosamine, the enzyme was named N-acetyl-D-glucosamine oxidase (NagOx). In contrast to most known (fungal) carbohydrate oxidases, NagOx could be overexpressed in a bacterial host, which facilitated detailed biochemical and enzyme engineering studies. Steady state kinetic analyses revealed that non-acetylated hexoses were also accepted as substrates albeit with lower efficiency. Upon determination of the crystal structure, structural insights into NagOx were obtained. A large cavity containing a biochemically bound FAD, tethered via histidyl and cysteinyl linkages, was observed. Substrate docking highlighted how a single residue (Leu251) plays a key role in the accommodation of N-acetylated sugars in the active site. Upon replacement of Leu251 (L251R mutant), an enzyme variant was generated with a drastically modified substrate acceptance profile, tuned toward non-N-acetylated monosaccharides and disaccharides. Furthermore, the activity toward bulkier substrates such as the trisaccharide maltotriose was introduced by this mutation. Due to its advantage of being overexpressed in a bacterial host, NagOx can be considered a promising alternative engineerable biocatalyst for selective oxidation of monosaccharides and oligosaccharides.

PLOS COMPUTATIONAL BIOLOGY

Ten simple rules on how to develop a stakeholder engagement plan

Susanne Hollmann, Babette Regener, Janelle Bechta, Lesley Tobin, and Domènica D'Elia

Published: October 13, 2022 | <https://doi.org/10.1371/journal.pcbi.1010920>

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Abstract
To make research responsible and research outcomes meaningful, it is necessary to communicate our research and to involve as many relevant stakeholders as possible, especially in application-oriented, involving information and communication technology (ICT) research. Nowadays, stakeholder engagement is of fundamental importance to project success and achieving the expected impact and is often mandatory in a regulatory funding context. Ultimately, research and development can only be successful if people react positively to the results and benefits generated by a project. For the wider acceptance of research outcomes, it is therefore essential that the public is made aware of and has an opportunity to discuss the results of research undertaken through two-way communication (interpersonal communication with researchers). Responsible Research and Innovation (RRI), an approach that anticipates and assesses potential implications and societal expectations regarding research and innovation, aims to foster inclusive and sustainable research and innovation. Research and innovation processes need to become more responsive and adaptive to these grand challenges. This implies, among other things, the introduction of broader foreign and impact assessments for new technologies beyond their enunciated market benefits and risks. Therefore, this article provides a structured workflow that explains “how to develop a stakeholder engagement plan” step by step.

EP-pred: A Machine Learning Tool for Bioprospecting Promiscuous Ester Hydrolases

Ruite Xiang, Laura Fernandez-Lopez, Ana Robles-Martin, Manuel Ferrer, and Victor Guallar

Version 1 | Received: 2 September 2022 | Approved: 7 September 2022 | Online: 7 September 2022 (04:53:30 CEST)

How to cite: Xiang, R.; Fernandez-Lopez, L.; Robles-Martin, A.; Ferrer, M.; Guallar, V. EP-pred: A Machine Learning Tool for Bioprospecting Promiscuous Ester Hydrolases. *Preprints* 2022, 2022090100 (doi: 10.20944/preprints202209.0100.v1).

Abstract
When bioprospecting for novel industrial enzymes, substrate promiscuity is a desirable property that increases the reusability of the enzyme. Among industrial enzymes, ester hydrolases have great relevance for which the demand has not ceased to increase. However, the search for new substrate promiscuous ester hydrolases is not trivial since the mechanism behind this property is greatly influenced by the active site's structural and physicochemical characteristics. These characteristics must be computed from the 3D structure, which is rarely available, and expensive to measure, hence the need for a method that can predict promiscuity from a sequence alone. Here we report such a method called EP-pred, an ensemble binary classifier, that combines three machine learning algorithms: SVM, kNN, and a Linear model. EP-pred has been evaluated against the Lipase Engineering Database together with a hidden Markov approach leading to a final set of 10 sequences predicted to encode promiscuous esterases. Experimental results confirmed the validity of our method since all ten proteins were found to exhibit a broad substrate ambiguity.

Keywords
biocatalysts; bioprospecting; esterases/lipases; hydrolases; machine learning; supervised learning

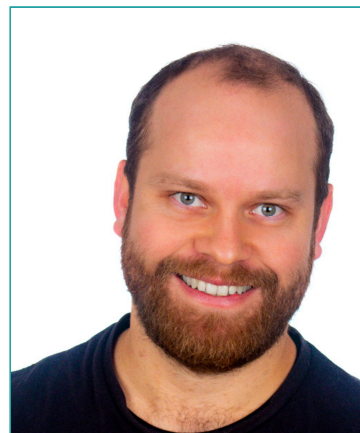
Who's new in team OXIPRO?

Welcome to our new researchers

The OXIPRO team at Barcelona Supercomputing Centre is delighted to welcome a new team member, Martin Floor. Born in the Netherlands, Martin was raised in Chile, where he successfully completed his BSc and MSc in Biochemistry at the University of Chile, followed by a PhD at the University of Vic in Catalonia.

In less than a year at BSC, he has succeeded in applying some of the theoretical concepts developed during his formative years to design new enzymatic systems computationally.

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OXIPRO is also delighted to introduce Rasmus Moen Ree, a new researcher who has joined the team at NORCE. Rasmus's research background is in molecular biology, which he studied at the University of Bergen, Norway. After successfully defending his PhD thesis in 2017, he has been working as a postdoctoral researcher in Bergen since then.

Within OXIPRO, Rasmus's aim is to test flavin-containing monooxygenases which have been engineered to adapt their cofactor requirements, as well as developing useful methods for analysing their reaction products.

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Research opportunities

The University of Groningen has announced 20 tenure-track position available for female researchers. The positions are for "women in industry, academia or research institutes who aspire to become a Full Professor in a European top research university."

Two positions are in OXIPRO partner [Marco Fraaije](#)'s research institute, Groningen Biomolecular Sciences and Biotechnology Institute (GBB), with foci on (1) Natural product discovery and engineering and (2) Cell factories for sustainable biosynthesis.

[Find out more...](#)



Synergies

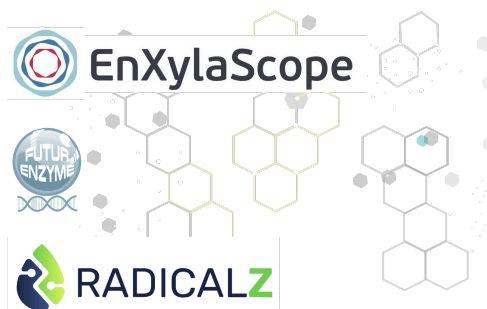
OXIPRO is closely working with ongoing research initiatives, in particular with our sibling projects funded under the same topic:

- [EnXylaScope](#)
- [FuturEnzyme](#)
- [Radicalz](#)

We're are about to issue our second newsletter: 'The Active Site'.

[Subscribe here](#) to receive news from all four projects, and find out more about our work.

OXIPRO's Sibling Projects



Forthcoming events

OXIPRO and/or our sister projects will be taking part in the following events where you can find out more about our work and activities undertaken by other biotech initiatives:

- [International Conference on Synthetic Enzyme Engineering and Applications \(ICSEEA\) \(Barcelona, Spain\)](#) 25/10/2022
- [Protein Engineering Congress \(Philadelphia, USA\)](#) 26-27/10/2022
- [Chicago IFT \(Chicago IL, USA\)](#) 01/11/2022
- [CPhI Europe \(Frankfurt, Germany\)](#) 01-03/11/2022
- [Enzyme Conference 2022 \(Oslo, Norway\)](#) 16-17/11/2022
- [Food Ingredients Europe \(Paris, France\)](#) 06-08/12/2022
- [Bioprospect 23 \(Norway\)](#) 14-16/03/2023
- [Novel Enzymes \(Greifswald, Germany\)](#) 28-31/03/2023
- [Biotrans 2023 \(La Rochelle, France\)](#) 25-29/06/2023

About OXIPRO

OXIPRO is a four-year initiative funded under the EU's Horizon 2020 programme and brings together a multidisciplinary team of researchers and stakeholders from 15 entities across Europe to focus on the development of novel enzymes for environment-friendly consumer products.

The OXIPRO partners are developing and deploying an efficient oxidoreductase foundry using cutting-edge bioinformatics and biotechnology, and by broadening the range of industrial oxidoreductases for more sustainable processes, this initiative will ultimately contribute to the transition to environment-friendly products, with detergents, textiles, sunscreens, and nutraceuticals.

Through the integration of computational workflows and state-of-the-art biotechnological technologies, OXIPRO will expedite the lab to market journey, while shortcutting downstream implementation and ensuring market uptake. This will be supported by ecosystem intelligence generated throughout the project as well as engagement with research, policy, societal and industrial actors in co-creation and interactions to maximise output and enable faster and systemic innovations.

For more information, contact:

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To join the OXIPRO Community and receive project updates, [please register here](#)

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