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Physics-based Machine Learning Models Predict Carbon Dioxide Solubility in Chemically Reactive Deep Eutectic Solvents

Background/Objective

- One promising approach for CO_2 capture is the utilization of deep eutectic solvents (DESs) as an ecofriendly and sustainable medium.
- Chemically reactive DESs are superior to nonreactive, physically based DESs

Approach

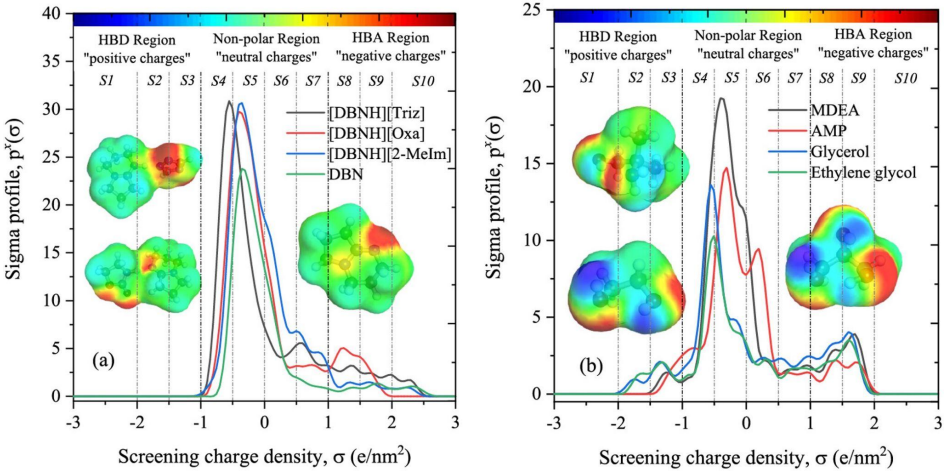
We collected 214 data points for the CO_2 solubility in 149 different chemically reactive DESs at different temperatures, pressures, and DES molar ratios from published work as a training set used by the machine learning (ML) models.

Results

An artificial neural network (ANN) provides the most accurate CO_2 solubility prediction with an average absolute relative deviation of 2.94% on the testing sets.

Significance/Impacts

This work provides ML models that can predict CO_2 solubility precisely and thus accelerate the design and application of chemically reactive DESs.



Representation of the ten *S*σ-profile descriptors in the σ-range for the (a) HBA and (b) HBD of DESs along with their COSMO cavities. The molecular polarity is graphically represented by the colors blue and red, where blue is the negative screening charge density ("*i.e.*, hydrogen bond donating capability"), while red represents the positive screening charge density ("*i.e.*, hydrogen bond accepting capability"). The green and yellow color regions characterize "neutral or nonpolar" molecular surfaces.

Mohan M., et. al. *ACS Omega.* doi: 10.1021/acsomega.4c01175

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Spatial Co-transcriptomics Reveals Discrete Stages of the Arbuscular Mycorrhizal Symbiosis

Background/Objective

We applied single-nuclei and spatial RNA sequencing to the arbuscular mycorrhizal symbiosis between *Medicago truncatula* and *Rhizophagus irregularis* to build a 2-D map of gene expression from both species

Approach

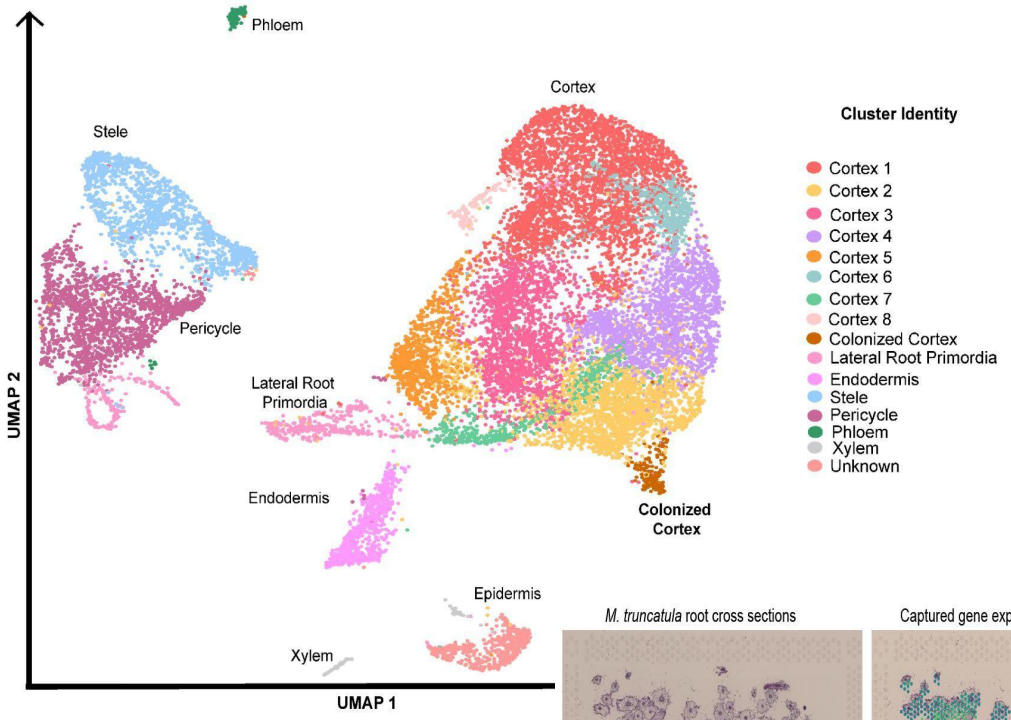
We analyzed the expression of known marker genes across datasets to map cells experiencing symbiosis across time and space and used that information to predict new genes involved in the interaction.

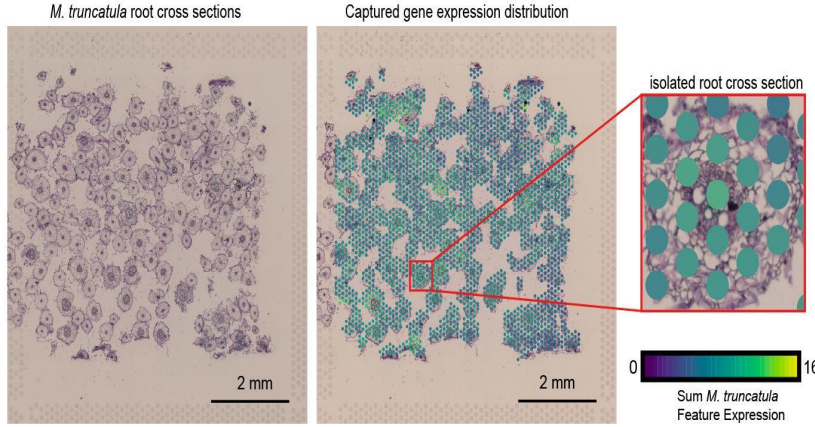
Results

We identified hundreds of novel *M. truncatula* and *R. irregularis* as symbiosis-responsive and improved the amount of fungal symbiotic genes by over 12,000 genes.

Significance/Impacts

This was the first transcriptomics study that successfully captured the transcriptome of a multi-kingdom interaction simultaneously.





Serrano K.et. al, Nature Plants. Doi: 10.1038/s41477-024-01666-3

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Genome-scale model development and genomic sequencing of the oleaginous clade Lipomyces

Background/Objective

- Lipomyces have become attractive candidates for renewable biofuel and chemical production from waste feedstocks
- A more comprehensive genome-scale metabolic model (GSM) can provide further understanding of metabolism and allows for comparisons of reactions with GSMs of other species

Results

A GSM of Lipomyces starkeyi NRRL Y-11557 was built using orthologous protein mappings to model yeast species

Significance/Impacts

- The developed GSM is a useful tool that can be used in combination with computational strain design algorithms to identify strategies for engineering and improving production strains.
- The model provides a more comprehensive map of L. starkeyi metabolism.

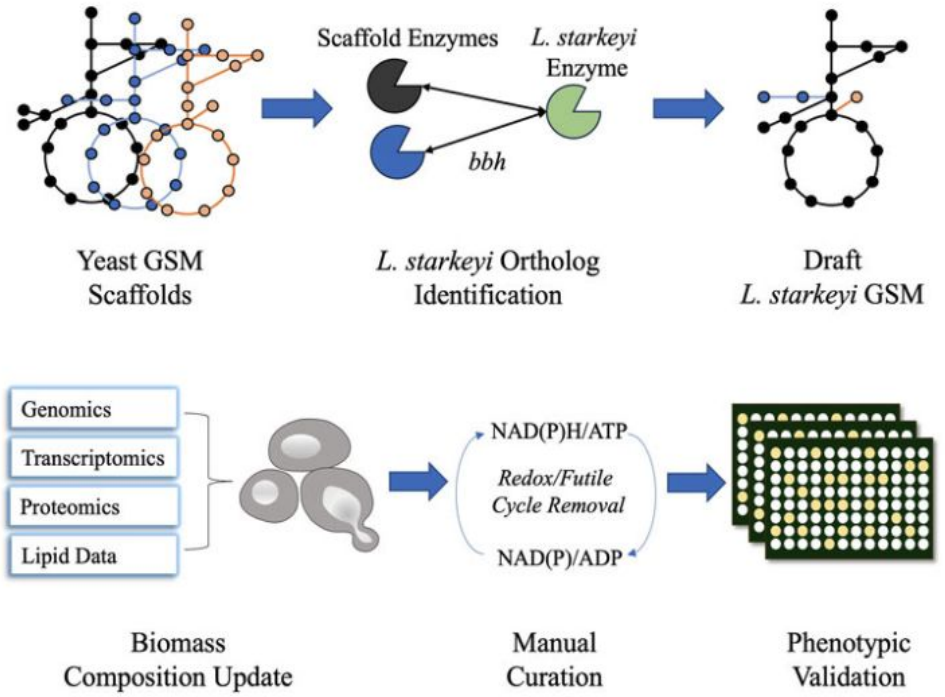

Figure 1. Schematic diagram of iLst996 genome-scale metabolic model (GSM) construction. Lipomyces starkeyi orthologs were identified using the NCBI blast tool for bidirectional best hits (bbhs) and the OrthoMCL pipeline. Orthologs were identified in three other yeast GSMs and were used to develop the initial draft GSM. The biomass composition and lipid synthesis reactions were then updated using L. starkeyi omics and lipid data. Manual curation was performed to remove futile cycles, leading to realistic flux predictions. Phenotypic microarray plates were then used to assess the accuracy of the model.

Czajka J. J. et. al. , Frontiers in bioengineering and biotechnology. doi: 10.3389/fbioe.2024.1356551

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Perspective on Lignin Conversion Strategies That Enable Next Generation Biorefineries

Background/Objective

- An urgent need lies in the design of an upstream chemical depolymerization process to achieve a higher titer of biocompatible and bioavailable molecules with a narrow product distribution profile
- From the bioconversion perspective, it is important to engineer existing enzymatic and microbial processes to enhance the utilization of a wider variety of lignin-derived monomers and/or oligomers

Approach

- We highlight the possibility of using synthetic co-culture and microbial hosts from extreme environmental conditions (extremophiles)
- We also emphasize dedicating significant research to the complex lignin-derived streams rather than using model compounds to better understand the behavior and metabolic pathways of the microbial host under actual considerations

Significance/Impacts

- Improved cost-effectiveness, carbon efficiency, and energy efficiency of the lignocellulosic biorefineries for renewable chemicals and materials
- Decarbonized bioeconomy by enabling lignin utilization efficiency

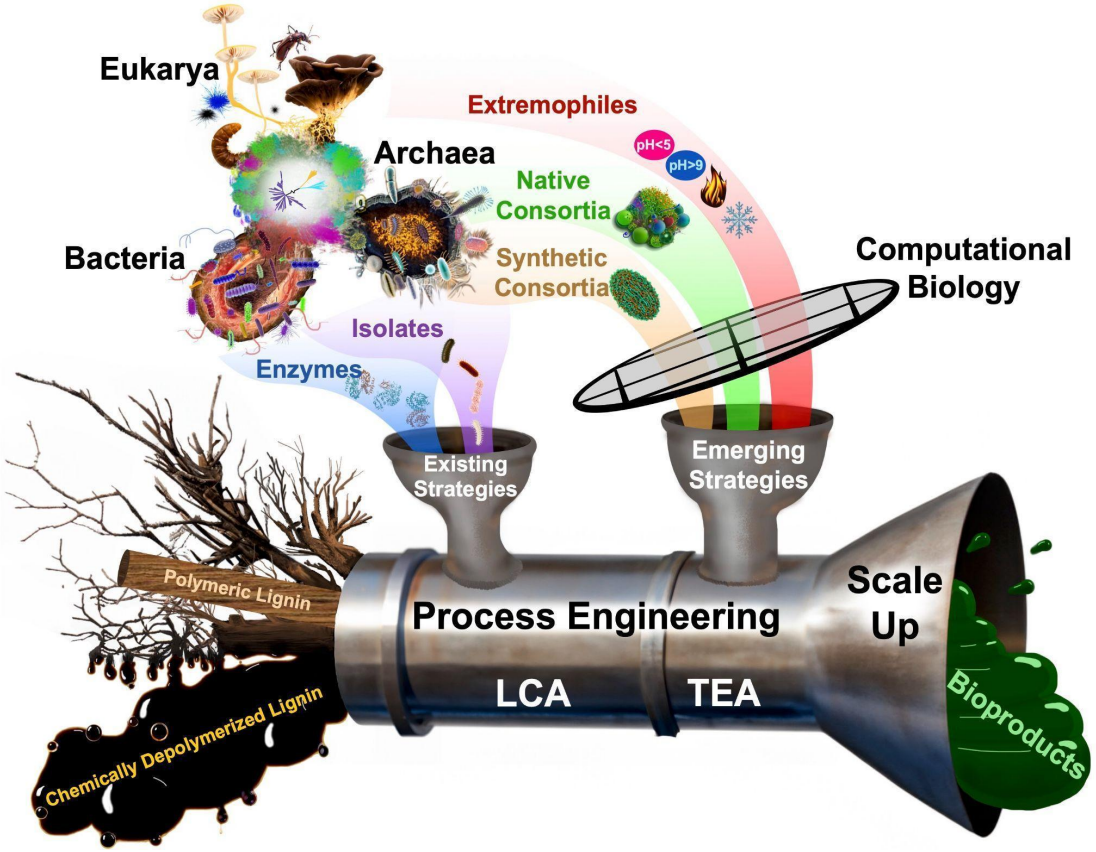

Figure. Schematic representation of existing and emerging biological approaches for lignin conversion to high-value bioproducts guided by process engineering, life cycle assessment, and techno-economic analysis to enable next-generation biorefineries.

Shrestha S., et. al. *ChemSusChem.* 10.1002/cssc.202301460

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Kinetic Analysis of the Hydrodeoxygenation of Aliphatic Volatilized Lignin Molecules on Bulk MoO_3: Elucidating the Formation of Alkenes and Alkanes

Background/Objective

- Working to derive value from the lignin portion
- MoO_3 has been found to be effective for the hydrodeoxygenation of lignin derivatives giving aromatics, alkenes and alkanes
- Desirable not to generate alkanes

Approach

Extensive kinetic analysis of model compounds to understand the mechanism for deoxygenation of oxygenated aliphatics.

Results

Detailed reaction mechanism identified for acetone dehydrogenation, which was extended to additional oxygenated aliphatics. Selectivity to alkanes was controlled by the electron donating nature of the groups next to the C-O bond.

Significance/Impacts

Alkenes and alkanes were generated in parallel rather than sequential, so further catalyst development is required,

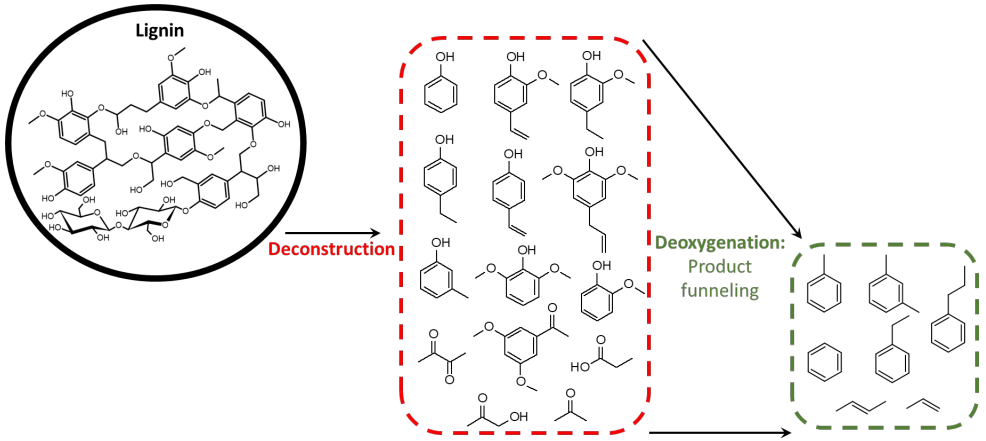

Figure 1: Funneling of lignin derivatives via deoxygenation to chemicals that can be directly introduced into the petrochemical industry.

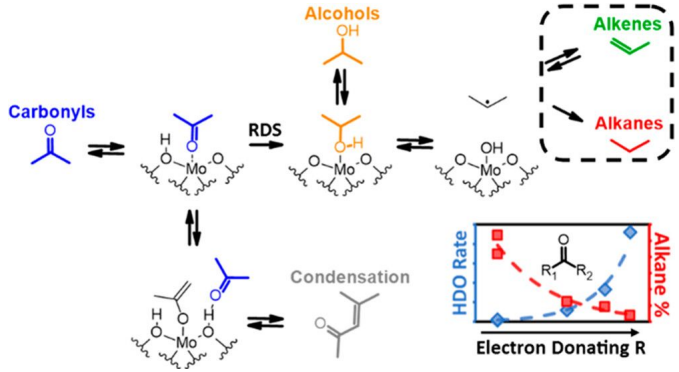

Figure 2: Acetone/propanol deoxygenation reaction network developed and extended to a range of oxygenated aliphatics.

Kohler, A.J., Walter, C.H., Shanks, B.H., ACS Catalysis, 13, 14813-14827 (2023) doi: 10.1021/acscatal.3c04444

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The short-and long-run environmental value of waste conversion

Background/Objective

- Develop recommendations for greenhouse gas accounting when biofuels and bioproducts are produced from waste products (e.g., crop residue)
- Establish guidance for distinguishing between waste and a product

Approach

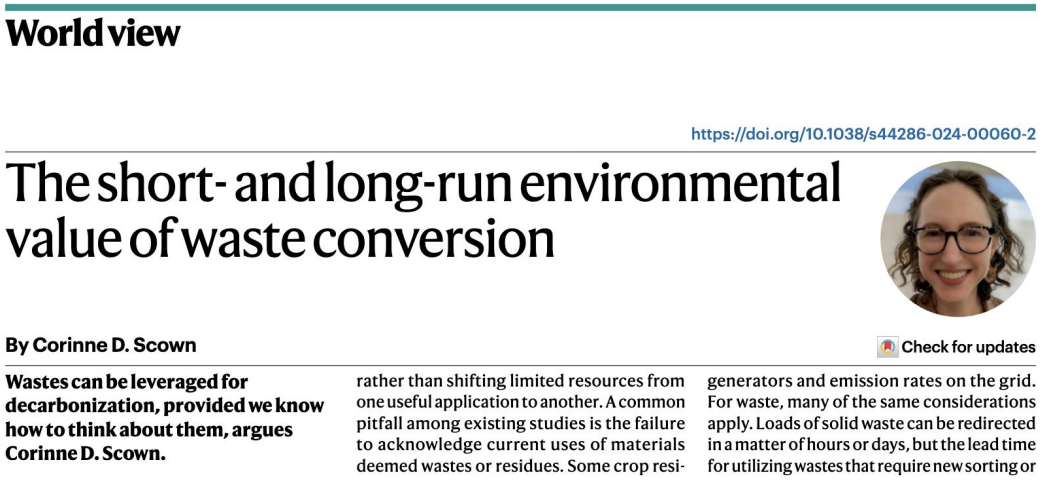
Develop a framework for distinguishing between wastes and products, and developing the counterfactual scenario for the material (what would have happened to it, absent its diversion to bioenergy/bioproducts)

Results

Proposed a differentiation between short- and long-run counterfactuals and GHG footprints/offsets for wastes.

Significance/Impacts

Implications for LCA researchers, clean fuel policy, and voluntary carbon markets



World view

https://doi.org/10.1038/s44286-024-00060-2

The short- and long-run environmental value of waste conversion

By Corinne D. Scown

Check for updates

Wastes can be leveraged for decarbonization, provided we know how to think about them, argues Corinne D. Scown.

rather than shifting limited resources from one useful application to another. A common pitfall among existing studies is the failure to acknowledge current uses of materials deemed wastes or residues. Some crop resi-

generators and emission rates on the grid. For waste, many of the same considerations apply. Loads of solid waste can be redirected in a matter of hours or days, but the lead time for utilizing wastes that require new sorting or

Scown, C.D. Nature Chemical Engineering. doi: 10.1038/s44286-024-00060-2

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Biosynthesis of Strained Amino Acids by a PLP-Dependent Enzyme through Cryptic Halogenation

Background/Objective

- Generating cyclopropane rings via chemical processes is challenging & requires the use of highly reactive chemical species
- Bes-D-like halogenases enable the biosynthesis of non-canonical amino acids (ncAAs) containing structural features of interest, like cyclopropanes, in specialty chemical production via cryptic halogenation. These enzymes are a recent discovery.

Approach

Bioinformatic identification of a biosynthetic pathway in the bacteria *Pseudomonas azotoformans* which formed a cyclopropane ncAA enabled characterization of its formation and application via LCMS, 2-D NMR, and genetic approaches

Results

PazA (halogenase) & PazB (cyclopropanase) enzymes form a new cyclopropane ncAA, pazamine. Use of PazB with other halogenases enabled production of other structures of interest. Pazamine-producing bacteria demonstrated potential impacts on hormonal function in plants

Significance/Impacts

Considerably broadens the enzymatic toolbox for biocatalytic production of specialty chemicals. Potential application in agricultural biotechnology as inhibitor of stress-induced ethylene

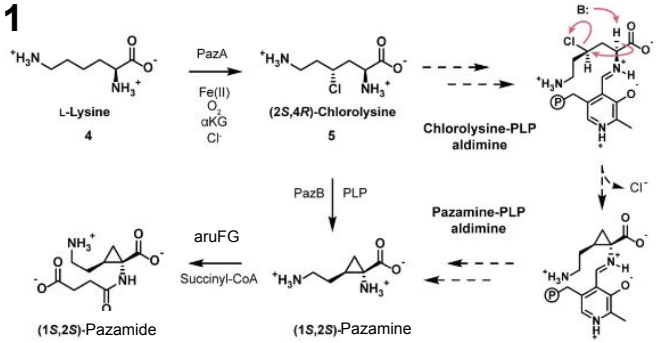

Figure 1: Proposed biosynthetic pathway to pazamine and pazamide

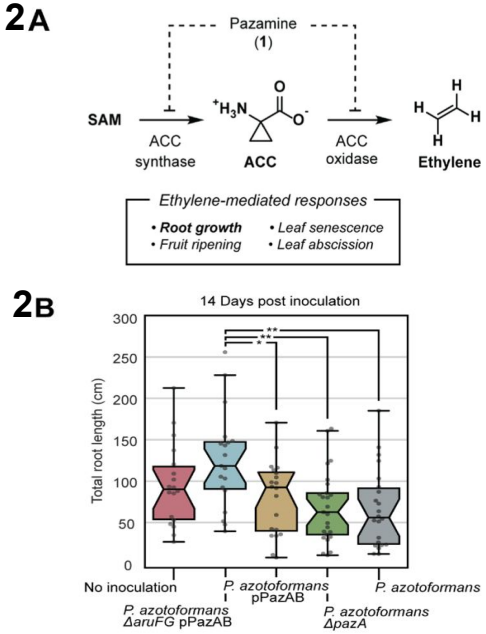

Figure 2: A) Pazamine is very similar to the ethylene precursor ACC and may be able to inhibit enzymes involved in plant ethylene biosynthesis. B) Inoculation of *Arabidopsis thaliana* with *P. azotoformans ΔaruFG pPazAB,* modified to increase pazamine production, rescues the short root phenotype caused by bacterial inoculation and subsequent ethylene production

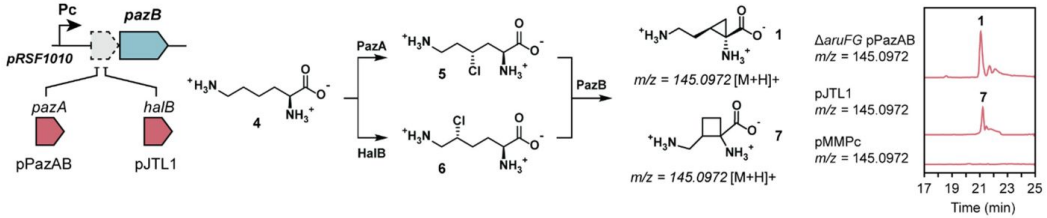

Figure 3: Combinatorial use of PazB enables biosynthetic production of new carbocycle-containing amino acids

Sosa M.B., et. al. *Angew. Chem. Int. Ed.* Doi: doi.org/10.1002/anie.202319344

ENABLED PUBLICATIONS

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Yeast Platforms for Production and Screening of Bioactive Derivatives of Rauwolscine

Background/Objective

- Monoterpene indole alkaloids (MIAs) are a highly bioactive class of metabolites produced by a range of plants.
- The corynanthe-type MIAs are a stereochemically complex subclass with therapeutic potential.

Approach

- We developed yeast-based cell factories for production of rauwolscine, yohimbine, tetrahydroalstonine, and corynanthine.

Results

- We demonstrate regioselective biosynthesis of 4 fluorinated derivatives of these compounds.
- We produced derivatives of these bioactive scaffolds.

Significance/Impacts

- This study demonstrates a discovery pipeline for bioactive plant-inspired small molecules based on one-pot biocatalysis of natural and new-to-nature corynanthe-type MIAs in yeast.

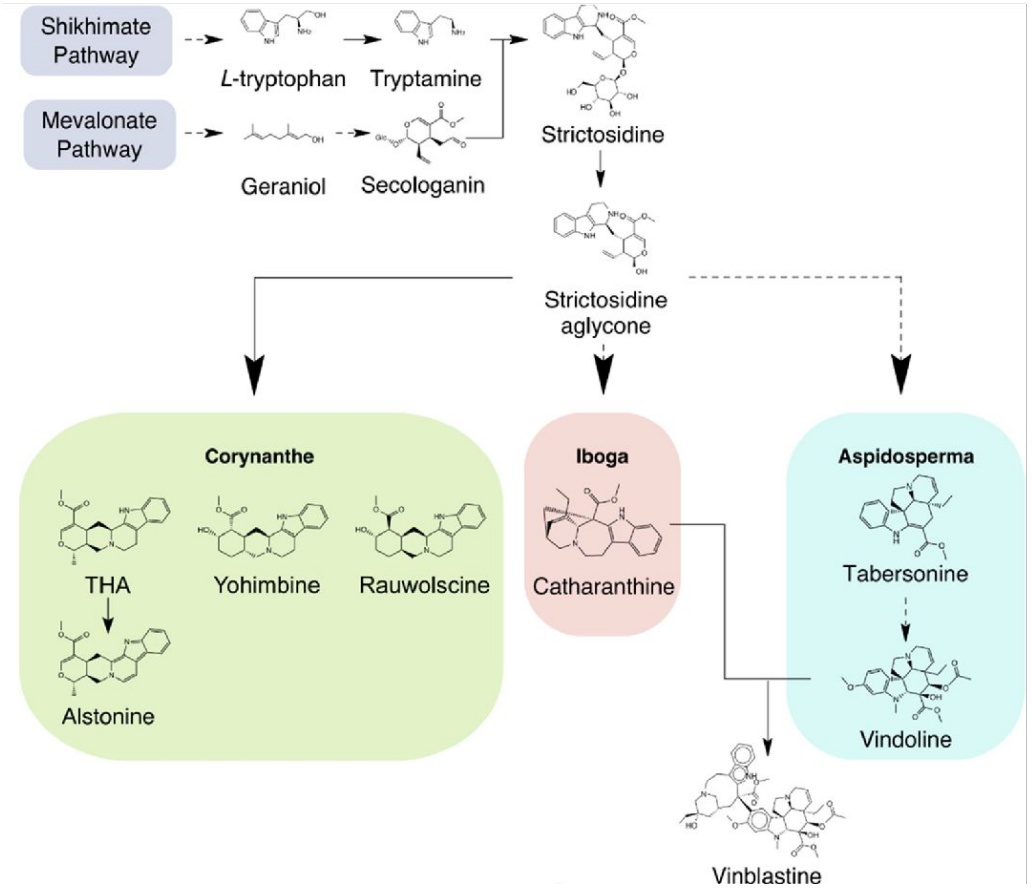

Figure 1. Key biosynthetic reactions of MIAs. Schematic outlining the key branch points in the MIA pathway. Examples of the three major classifications of MIA compounds in green (corynanthe), red (iboga), and blue (aspidosperma) boxes.

Bradley S. A., et. al. ACS synthetic biology. doi: 10.1021/acssynbio.4c00039

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Elucidation of genes enhancing natural product biosynthesis through co-evolution analysis

Background/Objective

- Streptomyces has the largest repertoire of natural product biosynthetic gene clusters (BGCs).
- Developing a universal engineering strategy for each Streptomyces species is challenging.

Approach

- We proposed that a set of genes co-evolved with BGCs to support biosynthetic proficiency must exist in those strains, and that their identification may provide universal strategies to improve the productivity of other strains.

Results

- When the pyrroloquinoline quinone (pqq) gene cluster was engineered into 11 Streptomyces strains, it enhanced production of 16,385 metabolites up to 40-fold improvement and several activated silent gene clusters.

Significance/Impacts

- This study provides an engineering strategy for improving polyketide production and finding previously unidentified BGCs.

Wang X., et. al. Nature metabolism. doi: https://doi.org/10.1038/s42255-024-01024-9

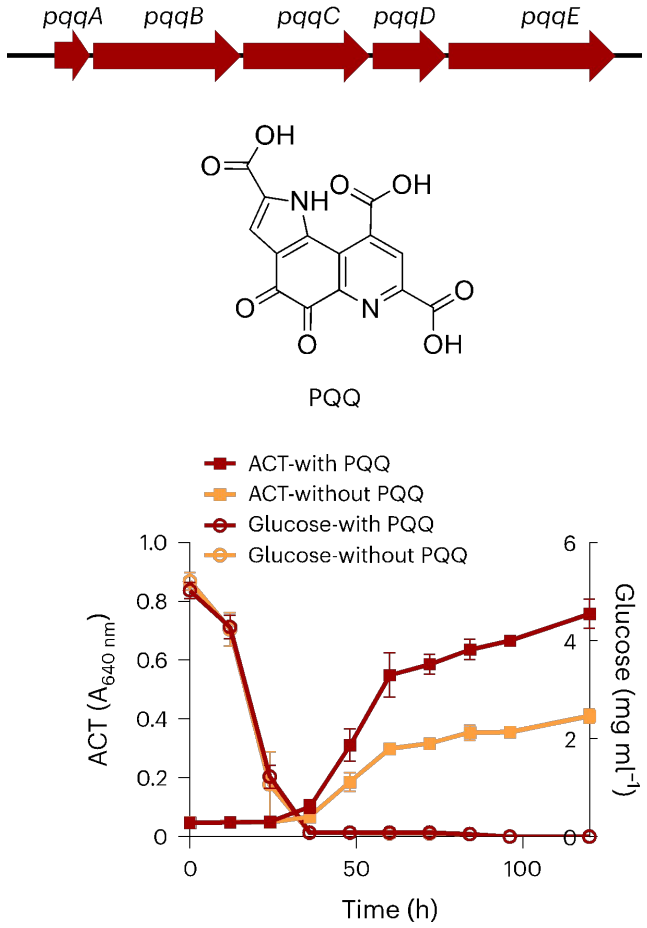

Figure 1. Top: PQQ and its biosynthetic gene cluster. Bottom: Actinorhodin production and glucose consumption in the presence and absence of the PQQ biosynthetic gene cluster.