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Economic and Environmental Trade-Offs of Simultaneous Sugar and Lignin Utilization for Biobased Fuels and Chemicals.

Background/Objective

Utilization of lignin is key to increasing the carbon conversion efficiency for bioenergy and reducing the amount of residual organic material that must be burned or treated

Approach

We built TEA and LCA models to quantify the tradeoffs between combusting lignin for electricity versus depolymerizing lignin and microbially converting monomers downstream

Results

Deconstructing lignin to bioavailable intermediates and utilizing those small molecules alongside sugars to boost product yields is economically attractive if the overall lignin-to-product conversion yield exceeds 11–20% by mass

Significance/Impacts

The performance thresholds for economic viability are ambitious but achievable, and are easier to meet for high-lignin feedstocks

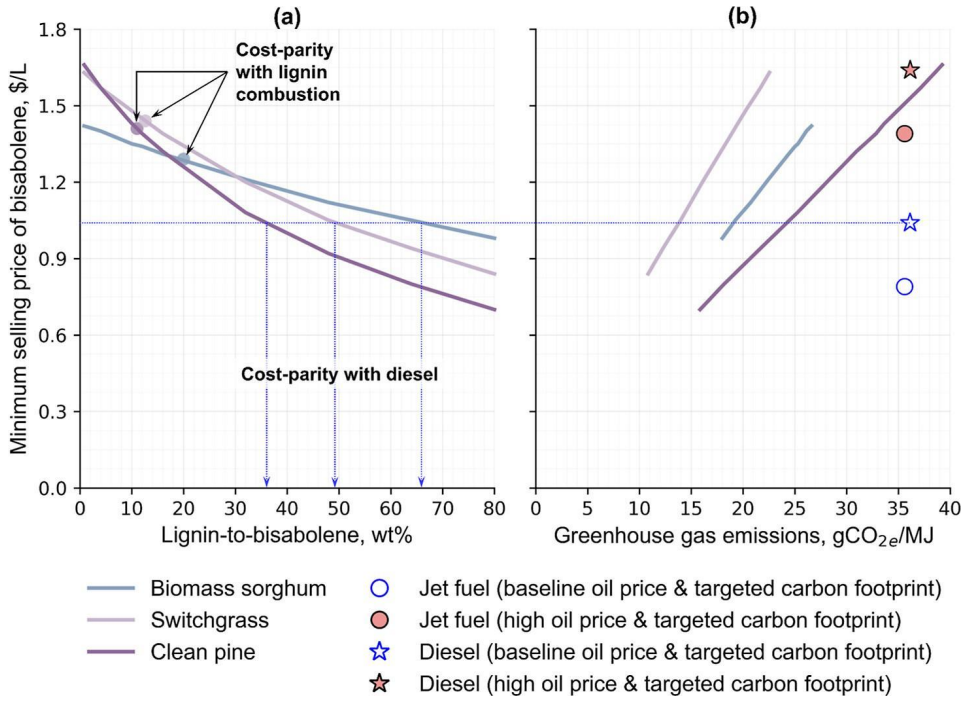

Figure 1: Minimum selling price of bisabolene as a function of (a) lignin to bisabolene conversion and (b) GHG emissions of bisabolene. The targeted carbon footprint of bisabolene aims for a 60% reduction relative to petroleum. All prices are presented in 2022$. Projected petroleum prices in 2050 (2022$) were gathered from Annual Energy Outlook 2023.

Baral N.R., et. al. ACS Sustainable Chemistry & Engineering. doi: 10.1021/acssuschemeng.3c05541

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Biomass pretreatment with distillable ionic liquids for an effective recycling and recovery approach

Background/Objective

We set out to construct a new process for recovering ionic liquids (ILs) within the context of biorefining that overcomes some of the existing drawbacks presented by conventional "water washing" and "one-pot" methods.

Approach

Compared different distillable protic ionic liquids and their alkanolamine analogues in terms of pretreatment efficiency and solvent recovery and recycle.

Results

We determined that 85% of ethanolamine acetate ([EthA][OAc]) could be recovered out of biomass while achieving 73.6% and 51.4% of theoretical glucose and xylose yields, respectively. Surprisingly, we found that ethanolamine produced higher sugar yields as well as higher solvent recoveries than [EthA][OAc].

Significance/Impacts

TEA found that distillation pressure played a decisive role in process economics, which revealed that applying only 47 % of vacuum would generate results that outperform the current state of the art.

Achinivu E.C., et al. Chemical Engineering Journal. doi: 10.1016/j.cej.2023.147824

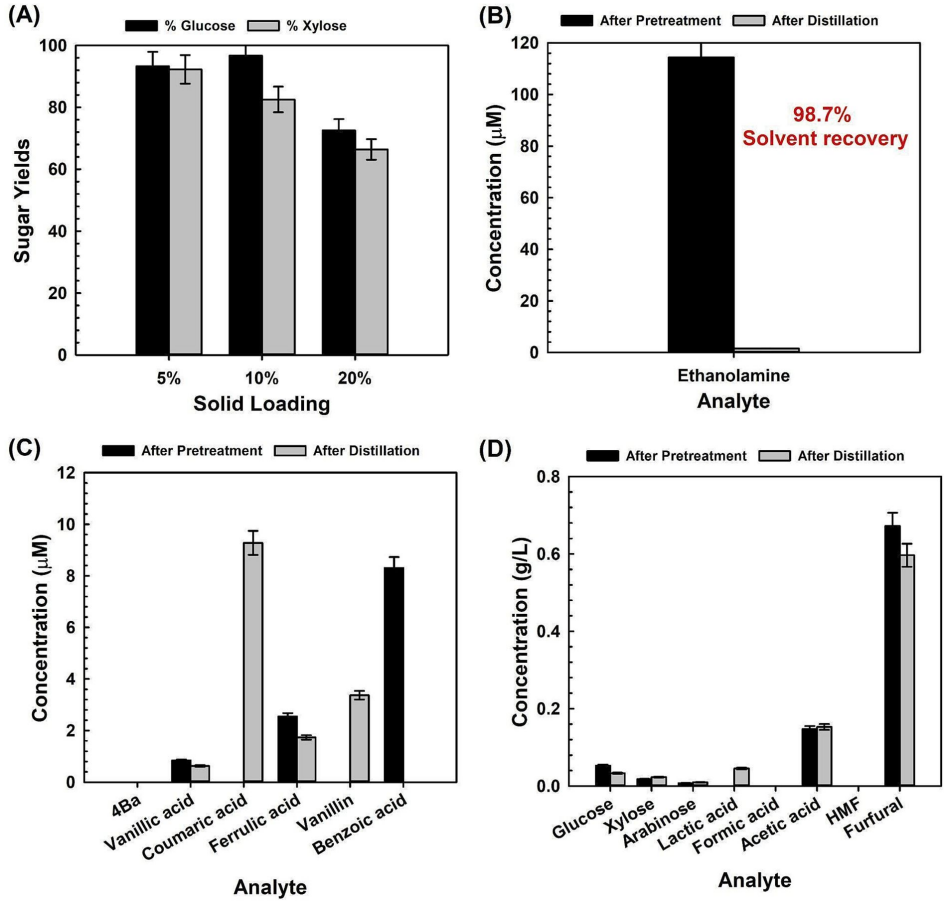

Figure 1: Conversion metrics for the organic solvent system (based on ethanolamine). A) Glucose and xylose yields with varying solid loading. B) Concentration of ethanolamine acetate immediately before and after distillation from biomass. C) Concentration of high value extractives before and after distillation D) Concentration of compounds of interest for fermentation before and after distillation.

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Characterization of the acoustic cavitation in ionic liquids in a horn-type ultrasound reactor

Background/Objective

The state of the art surrounding the characterization of acoustic cavitation in ionic liquids (ILs), a critical aspect of sonochemistry, is rather limited compared to that of aqueous working media.

Approach

We modelled an ultrasonic horn-type sonoreactor and investigated the effects of ultrasound power, sonotrode immersion depth, and solvent's thermodynamic properties on acoustic cavitation for 12 ILs.

Results

1-ethyl-3-methylimidazolium- and 1-butyl-3-methylimidazolium-based ILs yielded the largest active region volumes and the fastest acoustic jets.

Significance/Impacts

This study advances the understanding of acoustic cavitation behaviour in ionic liquids and provides valuable insights for optimizing ultrasound-assisted processes in these solvents, such as biomass pretreatment.

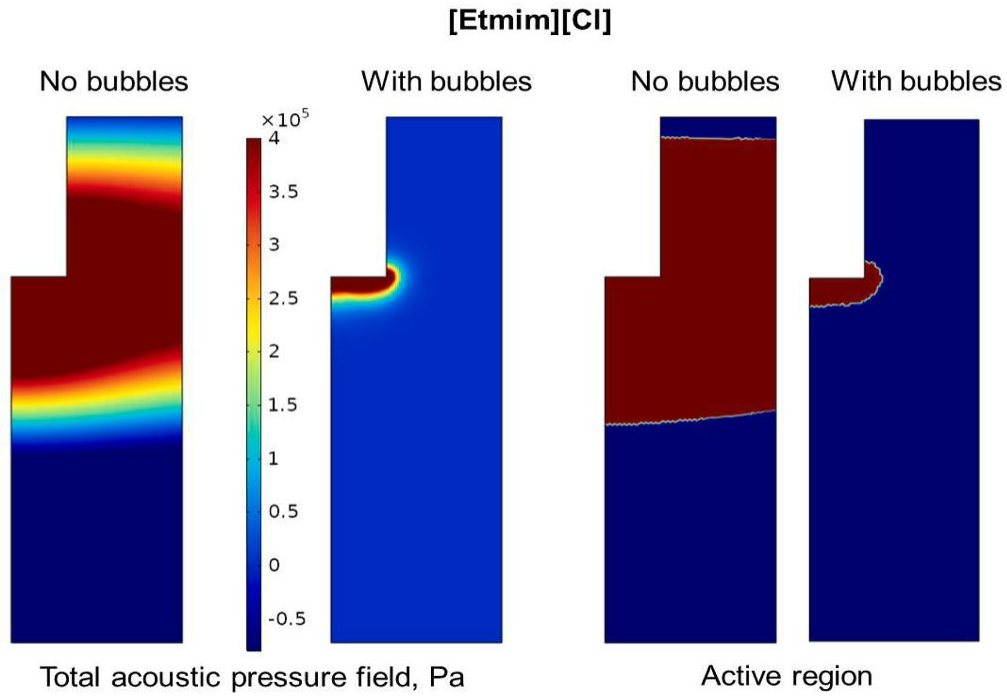

Figure 1: Profiles of acoustic pressure field and active volume regions for [Etmim][Cl] at 60 W andd = 2 cm. Comparison between simulations with (profiles on the right) and without (profiles on the left) acoustic attenuation elicited by cavitation bubbles. For [Etmim][Cl], the volumes of the active regions differ by 193 %.

Schieppati D., et. al. Ultrasonics Sonochemistry. doi: 10.1016/j.ultsonch.2023.106721

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Harnessing Plant Sugar Metabolism for Glycoengineering

Background/Objective:

We review how sugars are one of the fundamental building blocks of life, but despite their essentiality, only a limited number of polysaccharides and glycoconjugates can be made synthetically.

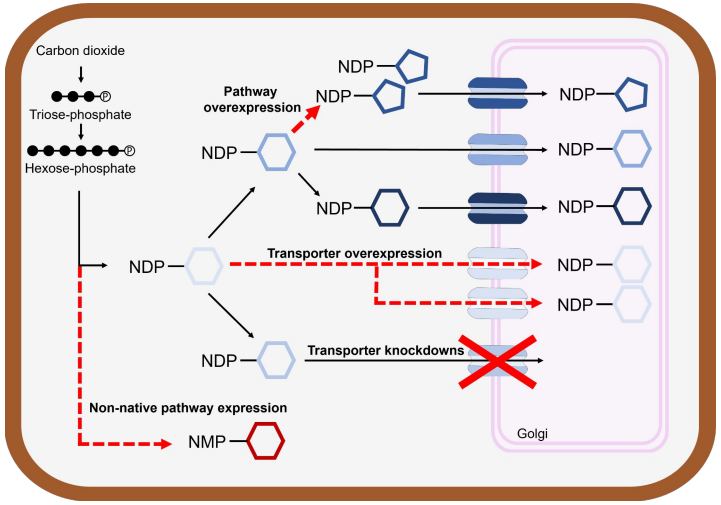
Results:

Plants use photosynthesis to produce a vast array of sugar-derived compounds in large quantities, while other means of production, such as chemical synthesis or microbial fermentation, are narrow in their range of sugar chemistries and comparatively low in yield. These qualities make plants an attractive platform for the synthesis of sugars and other glycosylated products.

Significance/Impacts : Plants have already been engineered to make products composed of or containing sugars that otherwise may be challenging to synthesize in other commonly used systems. Their growing use in glycoengineering efforts will continue to expand the production of diverse sugar-derived compounds.

Tang S.N., et. al. Biology. doi: 10.3390/biology12121505

A



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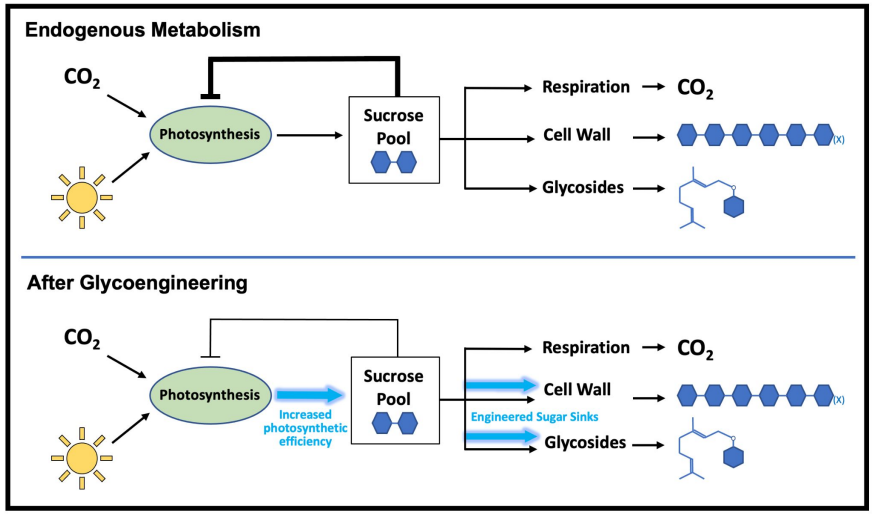

Figure 1: (A) Strategies for nucleotide sugar engineering. (B) Redirecting carbon in plants to sugar products

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Characterization and Diversification of AraC/XylS Family Regulators (AFRs) Guided by Transposon Sequencing

Background/Objective

- P. putida has diverse metabolisms → diverse regulators
- Regulators can be leveraged as biosensors and synbio tools

Approach

- RB-TnSeq data → identify potential ligands and promoters
- LBL Foldy → fold AFR & dock ligands, identify mutations
- Design and test constructs in both *E. coli and P. putida*

Results

- 11 promoters activated by specific inducers in *P. putida*
- 3 AFRs functioned in *E. coli*
- 1st reported AFR response to a –CoA (2-methylbutyrl-CoA)
- Expanded an AFRs inducer range from 3 lactams to 8 cyclic compounds

Significance/Impacts

- 2-methylbutyryl-CoA is a PKS substrate → potential for dynamic gene regulation or screening for high producers of similar –CoAs
- Lactams/lactones are flavors/fuels/fragrances/plastics; biosensors can aid in developing/improving bioproduction

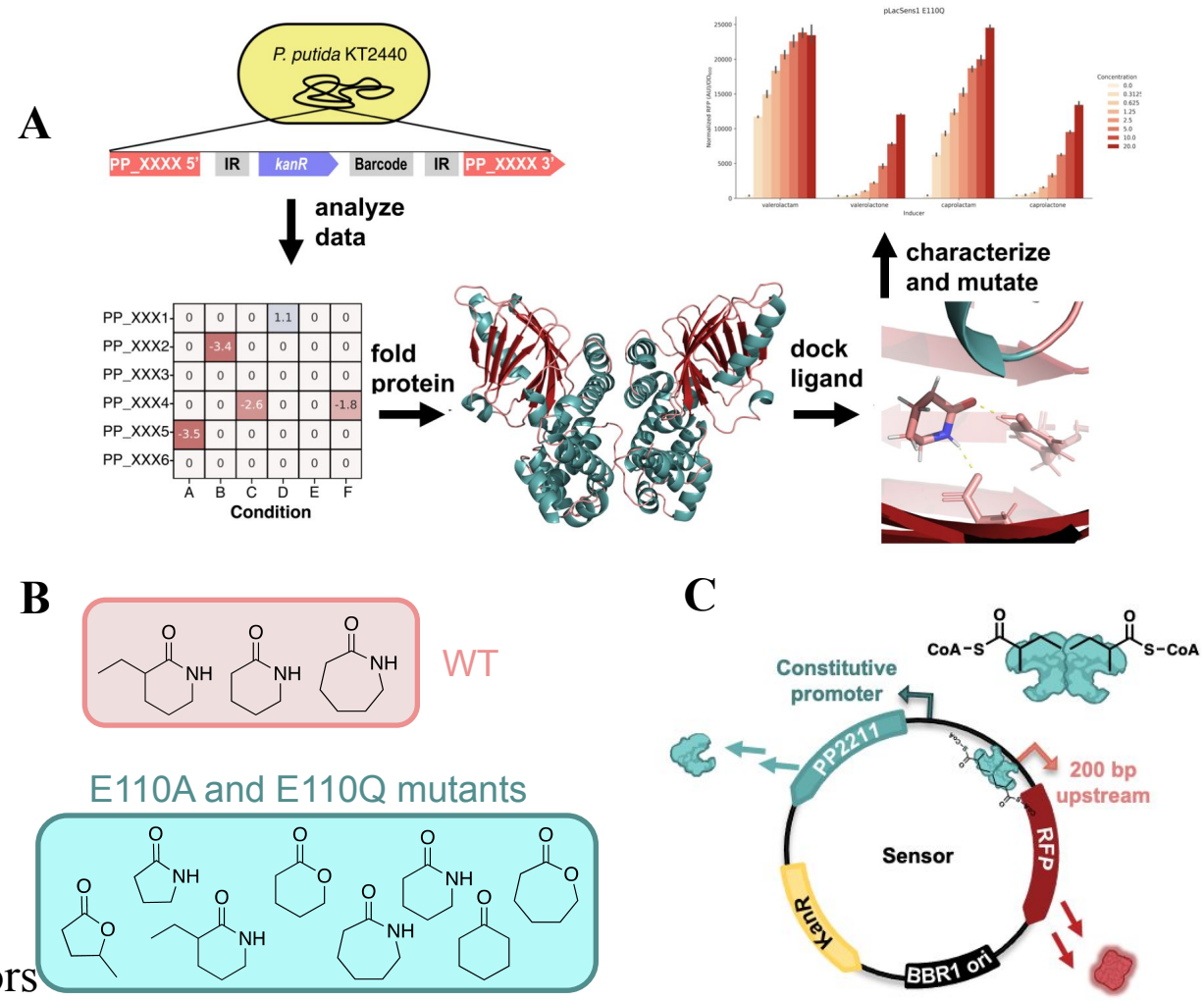

Figure: (A) Graphical overview of the research study. (B) Two mutants of OplR can detect 5 compounds that WT cannot C) PP2211 detects 2-methylbutyryl-CoA, the first reported AFR that senses a -CoA

Pearson A.N. and Incha M.I., et. al. (2023) ***ACS Synthetic Biology*****. doi: 10.1021/acssynbio.3c00441**

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Increased drought and extreme events over continental United States under high emissions scenario

Background/Objective

Objective: downscale climate data for US weather stations and analyze future trends in meteorological drought and temperature extremes, particularly during bioenergy crop growing seasons. This enables better yield predictions.

Approach

We used data from 4161 weather stations across the CONUS to downscale future precipitation projections from three ESMs participating in the CMIP6 SSP5 8.5.

Results

- Comparing historic observations with climate model projections revealed a significant bias in total annual precipitation days and total precipitation amounts.
- We expect an increase in the number of drought months in the future (2023–2052)

Significance/Impacts

- Drought-resistant bioenergy crops will be crucial for the bioeconomy

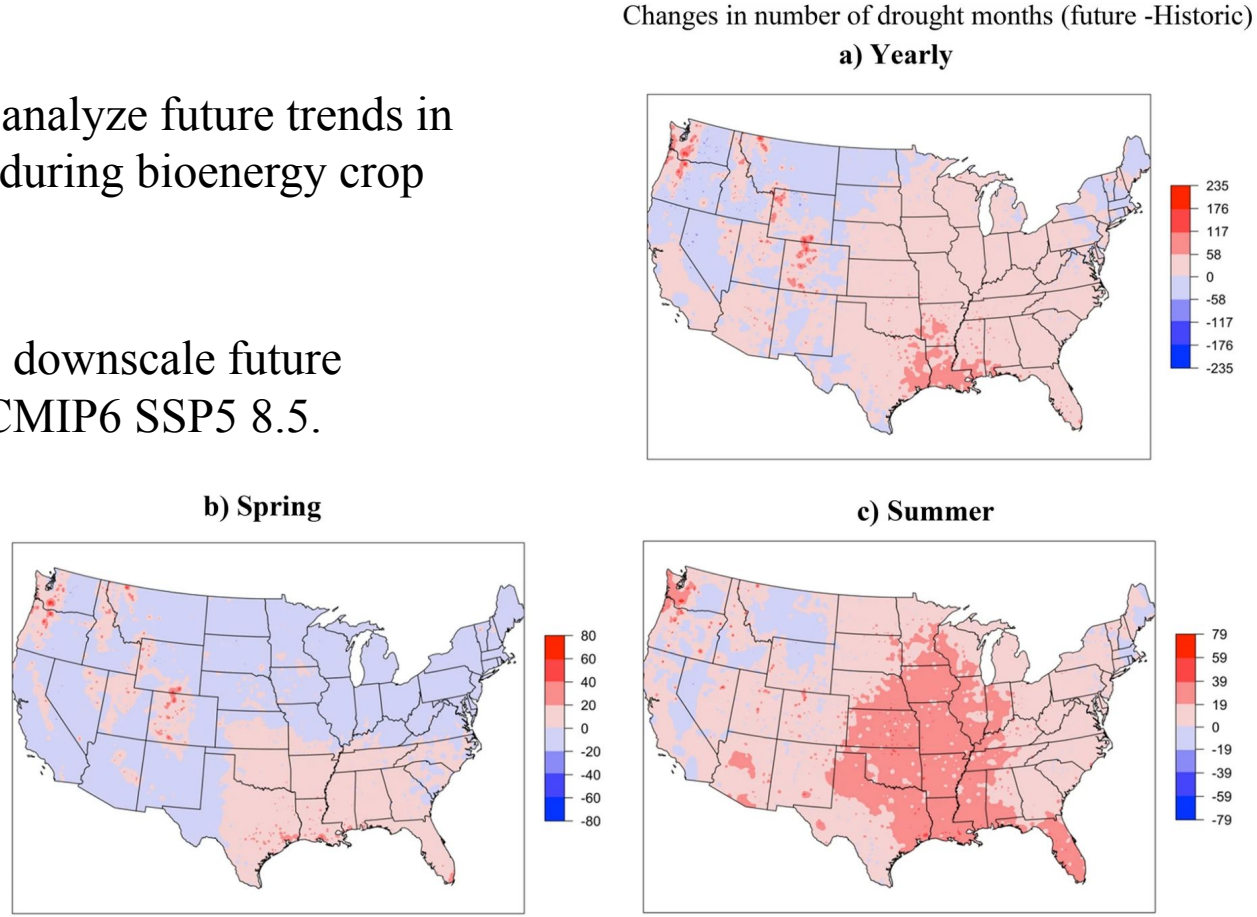

Figure 1: Comparison of change in drought months over 30-year period based on observation (1989–2018) and ensemble mean from the Earth system models future (2023–2052); yearly comparison (a), spring comparison (b) and summer comparison (c).

Gautam S., et. al. Sci Rep. doi: 10.1038/s41598-023-48650-z

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Development of Corynebacterium glutamicum as a monoterpene production platform

Background/Objective

- C. glutamicum, a GRAS and industrial workhorse organism, could be a potential host for effective monoterpene production

Approach

- Targeted genetic deletions and plasmid design iterations to 1) increase flux through the mevalonate-based bypass pathway, measuring isoprenol as a proxy for flux 2) increase flux to the desired monoterpenes
- Development of biphasic production system to address volatility

Results

- Highest reported isoprenol titers in *C. glutamicum* at 1.5 g/L
- Produced 321.1 mg/L of geranoids, 723.6 mg/L of 1,8-cineole, and 227.8 mg/L of linalool
- Elucidated aspects of the host oxidation/reduction of geranoids

Significance/Impacts:

Highest monoterpene titers in C. glutamicum to date is an important step towards developing it as an industrial GRAS monoterpene platform.

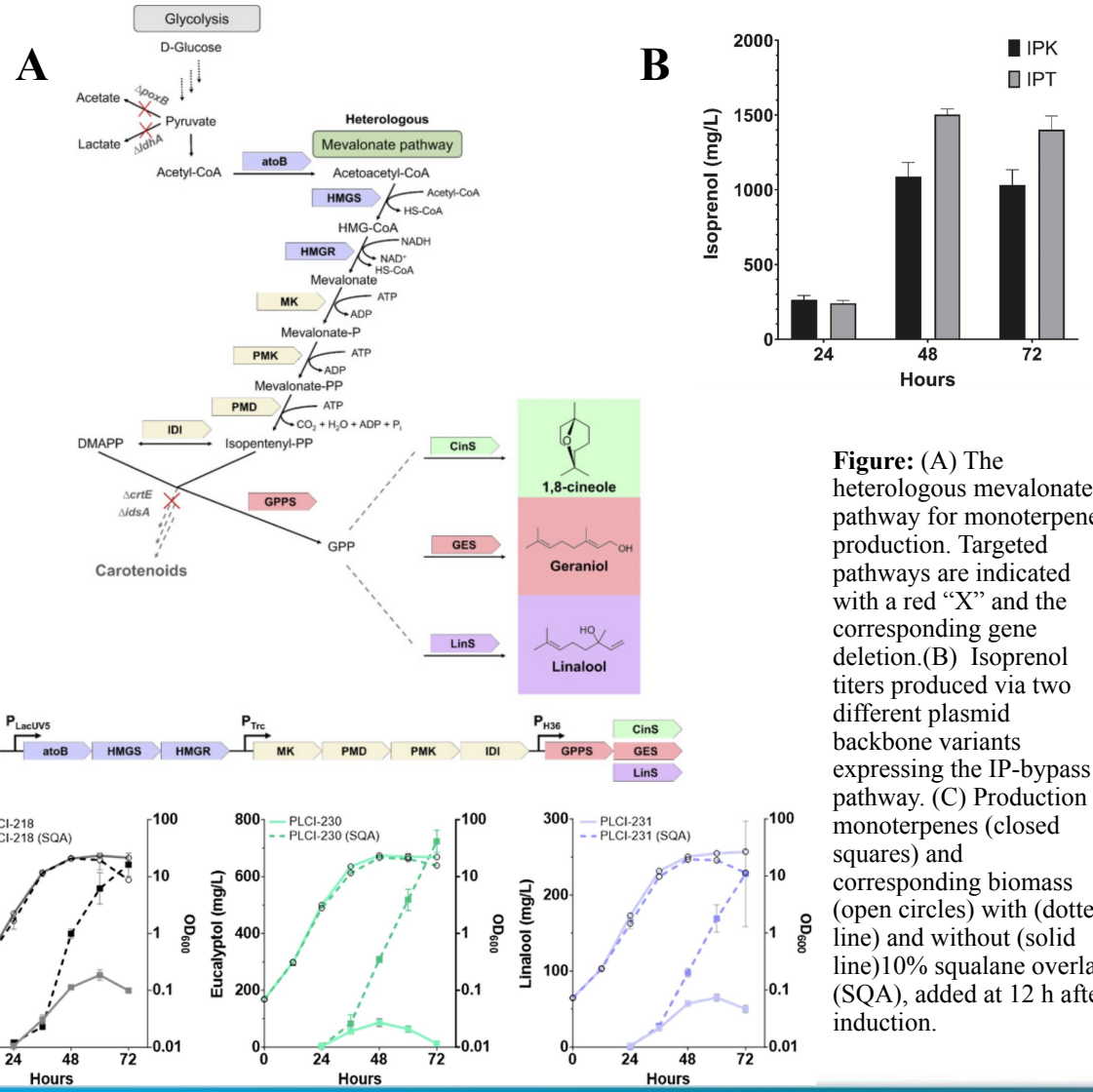

Figure: (A) The heterologous mevalonate pathway for monoterpene production. Targeted pathways are indicated with a red "X" and the corresponding gene deletion.(B) Isoprenol titers produced via two different plasmid backbone variants expressing the IP-bypass pathway. (C) Production of monoterpenes (closed squares) and corresponding biomass (open circles) with (dotted line) and without (solid line)10% squalane overlay (SQA), added at 12 h after induction.

Luckie B.A., et. al. (2023) ***Metabolic Engineering*****. doi: 10.1016/j.ymben.2023.11.009**

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A large sequenced mutant library - valuable reverse genetic resource that covers 98% of sorghum genes

Background/Objective

- Sorghum is a multi-functional drought-tolerant C4 crop. It is also a DoE flagship bioenergy species.
- Mutant populations are critical for functional genomics, and the discovery of novel traits. They can also be planted directly in the field (non-GMO).

Approach

Here, in collaboration with the USDA, other BRCs, and the JGI we sequenced a large population of EMS-treated BTx623 *Sorghum bicolor*

Results

- We report coverage of 98% of annotated sorghum genes
- We also report 610 320 mutations within the promoter and enhancer regions of 18 000 and 11 790 genes respectively, providing an important resource for studying cis regulatory elements

Significance/Impacts

All mutations are searchable through Sorghumbase (https://www.sorghumbase.org/) and SorbMutDB (https://www.depts.ttu.edu/igcast/SorbMutDB.php) and seeds are available from the USDA

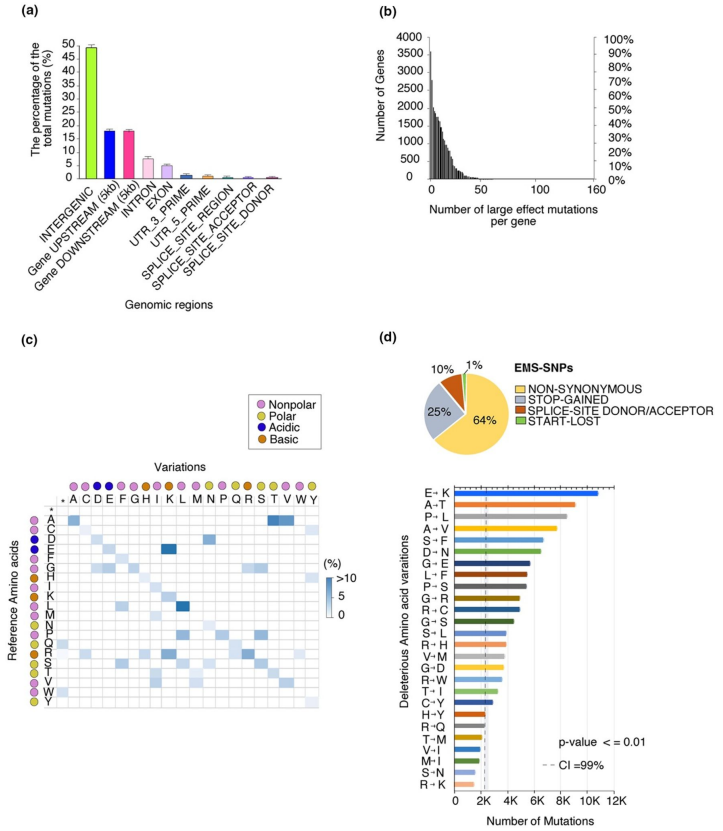

Figure 1: A summary of the mutations. (a) Distribution of ethyl methane sulfonate (EMS)-induced mutations in different genomic regions of the Sorghum Genome. The abundance is plotted in percent.(b) Distribution of the number of large effect mutations in genes.(c) Amino acid changes caused by EMS. The diagonal matrix shows the percent change (%) from one amino acid to another amino acid. The biochemical property of every amino acid is on the top. (d) A pie chart (upper panel) showing the distribution of high impact mutations in coding regions i.e., non-synonymous, stop-gained, splice-site donor/or acceptor, and start lost. The bar graph shows the frequency of the predicted deleterious mutations (SIFT score < 0.05) deleterious amino acid variation. The dotted line depicts a confidence interval of 99%.

Jiao Y., et. al. The Plant journal. doi: 10.1111/tpj.16582

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Impact of bioenergy feedstock carbon farming on sustainable aviation fuel viability in the United States

Background/Objective

- Sorghum, switchgrass, and Miscanthus are all deep-rooted, high-yielding biomass crops that can sequester soil carbon
- How soil carbon sequestration is accounted for will impact their viability as biofuel feedstocks

Approach

- DAYCENT models were developed to predict Miscanthus, sorghum, and switchgrass yields and CO_2, CH_4, and N_2O fluxes
- We modeled each feedstock's conversion to DMCO (a jet fuel)

Results

- If SOC accumulation is valued at \$185/ton CO_2, planting Miscanthus for conversion to DMCO would be economically cost-competitive across 66% of croplands. Cutting the SOC sequestration value in half reduces the viable area to 54%.

Significance/Impacts

- Combining agroecosystem and field-to-biofuel production process models reveals the impact of how we credit soil carbon sequestration

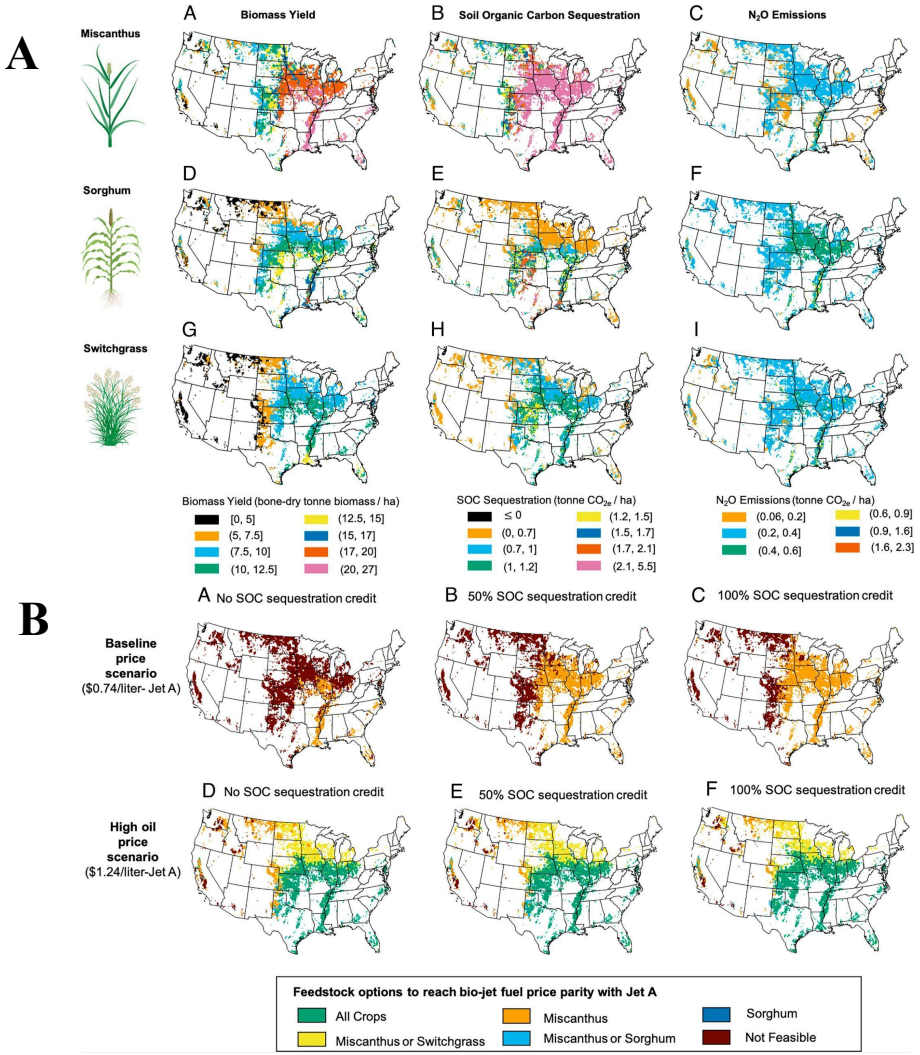

Figure 1: (A) Predicted yields for Miscanthus, sorghum, and switchgrass (B) Competitiveness of each crop as a SAF feedstock depending on how SOC is credited

Gautam S., et. al. Proceedings of the National Academy of Sciences of the United States of America. doi: 10.1073/pnas.2312667120

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Ten simple rules for managing laboratory information

Background/Objective

Information is the cornerstone of research, from experimental (meta)data and computational processes to complex inventories of reagents and equipment.

Approach

Develop and describe 10 simple rules discuss best practices for leveraging laboratory information management systems.

Results

10 rules are presented to help build strong foundations in laboratory information management to avoid the costly and frustrating mistakes.

Significance/Impacts

Best practices presented will help transform large information loads into useful scientific findings.

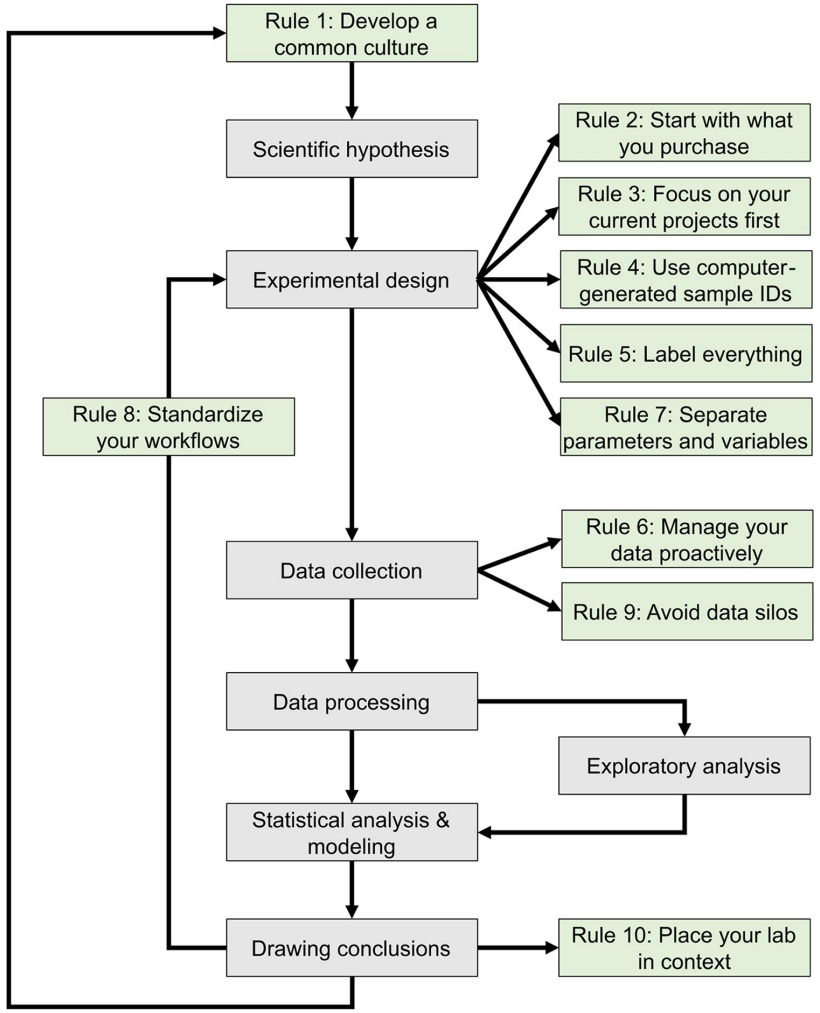

Figure 1: Information management enhances the experimental and modeling cycle

Berezin C.T., et. al. PLoS computational biology. doi: 10.1371/journal.pcbi.1011652

JBEI Enabled Papers

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UniKP: a unified framework for the prediction of enzyme kinetic parameters

Background/Objective

Prediction of enzyme kinetic parameters is essential for designing and optimizing enzymes for various biotechnological and industrial applications, but the limited performance of current prediction tools on diverse tasks hinders their practical applications.

Approach

We developed UniKP, a unified framework based on pretrained language models for the prediction of enzyme kinetic parameters from protein sequences and substrate structures.

Results

We have demonstrated the application of UniKP and EF-UniKP in several enzyme discovery and directed evolution tasks, leading to the identification of new enzymes and enzyme mutants with higher activity.

Significance/Impacts

UniKP is a valuable tool for deciphering enzyme kinetics and enables novel insights into enzyme engineering and their industrial applications.

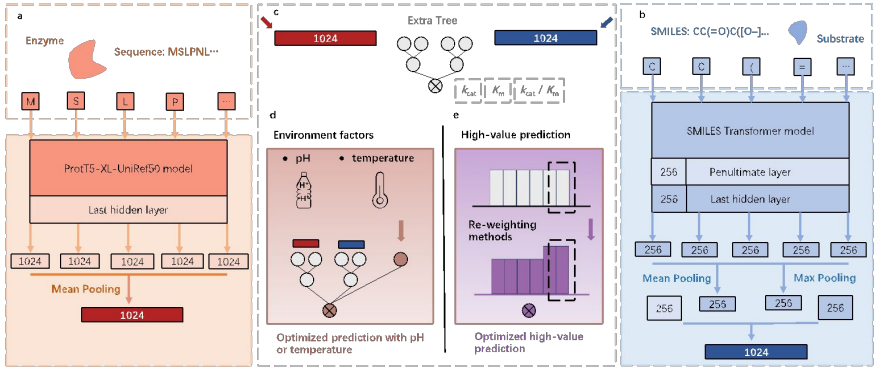

Figure 1: The overview of UniKP. a Enzyme sequence representation module. b Substrate structure representation module. c Machine learning module. d EF-UniKP. e Various re-weighting methods were used to adjust the sample weight distribution to generate an optimized prediction for high-value prediction task.

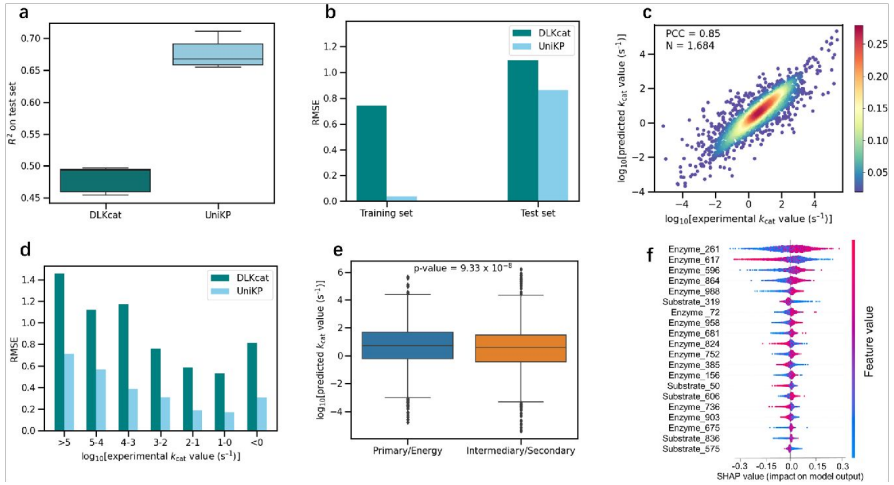

Figure 2: High accuracy of UniKP in enzyme kcat prediction.

Yu H., et. al. Nat Commun. doi: 10.1038/s41467-023-44113-1

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Corridor-Level Impacts of Battery-Electric Heavy-Duty Trucks and the Effects of Policy in the United States

Background/Objective

- TEA/LCA models struggle to capture the complexities of the evolving grid, including changes in hourly prices and net emissions impacts
- Linking these models with more sophisticated grid scenarios can address this issue

Approach

- We used grid scenarios developed by NREL, combined with plant-level emissions data to produce the "McGrid" model and demonstrate it in the context of freight truck electrification

Results

- The grid model allows for different externality costs to be placed on human health and climate impacts
- Most corridors can reduce health impacts from air pollution if electrified by 2040 recent tax incentives accelerate this to 2030

Significance/Impacts

- The grid model opens the possibility of analyzing the co-evolution of the grid with other industrial facilities, including biorefineries

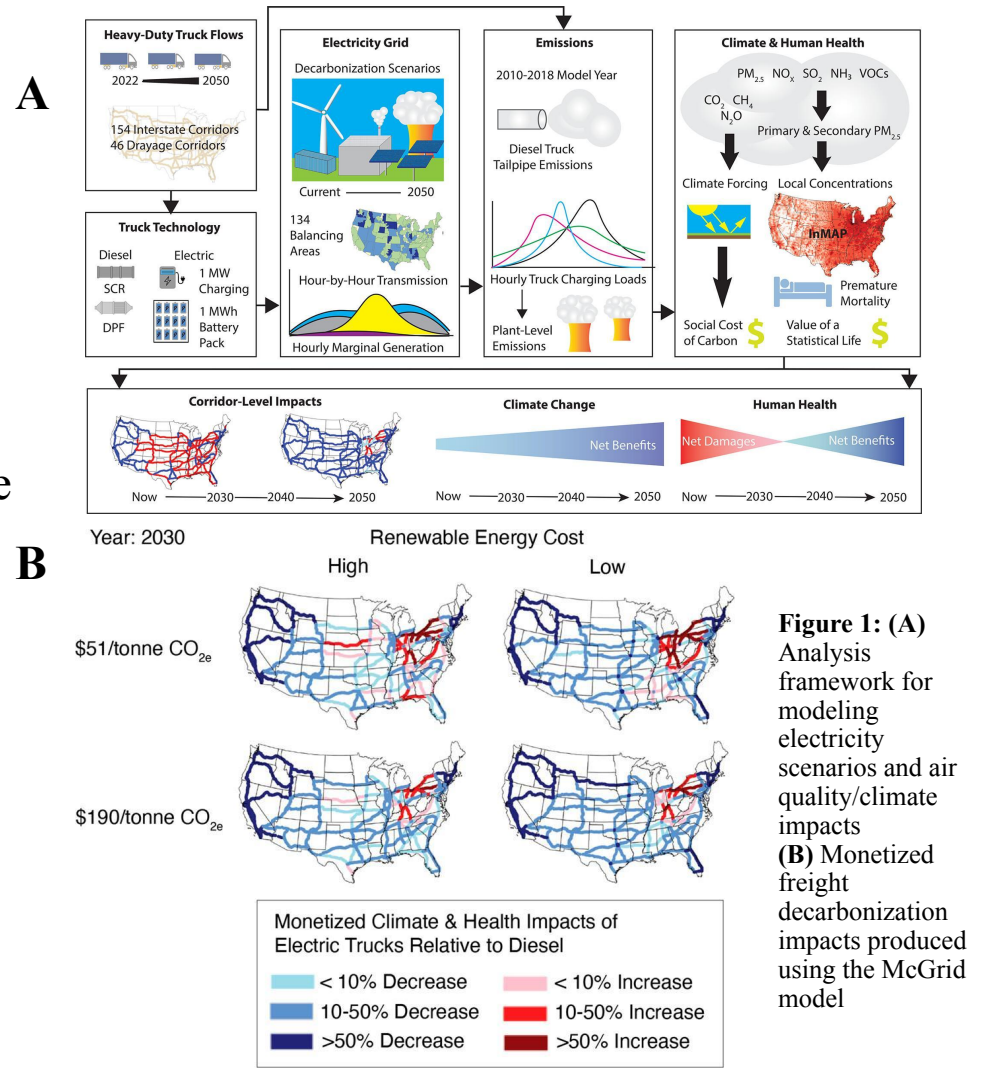

Figure 1: (A) Analysis framework for modeling electricity scenarios and air quality/climate impacts **(B)** Monetized freight decarbonization impacts produced using the McGrid model

McNeil W.H., et. al. Environmental science & technology. doi: 10.1021/acs.est.3c05139

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Shaping the future US bioeconomy through safety, security, sustainability, and social responsibility

Background/Objective

The US bioeconomy is currently valued at over US$950 billion and accounts for >5% of the gross domestic product.

Approach

This article describes how a group of bioindustrial manufacturing companies and researchers are conceptualizing the norms that should govern the field, to include safety, security, sustainability, and social responsibility

Results

Biomanufacturing practitioners and researchers describe the norms that should govern the growing, global field, to include safety, security, sustainability, and social responsibility. These '4S Principles' can ensure the field provides the greatest benefits to society.

4S Principles	4S Committee working definitions
Safety	Practices, controls, and measures taken to protect people and the environment from harm from biomanufacturing development process and/or physical products or byproducts. Includes safety of the workplace, consumers, and the general public.
Security	Measures taken across the biotechnology and biomanufacturing sectors including food and agriculture, materials, and energy, to manage potential threats and loss due to theft, misuse, diversion, unauthorized possession of property (including intellectual property) or intentional release of biological risk and/or technology.
Sustainability	Measures taken to maintain or improve the long-term viability of the environment and economy due to advancing biomanufacturing processes. These would include consideration of the impacts of products and processes on the environment, supply chains, as well as local public/consumer acceptance and practices.
Social responsibility	A principle that acknowledges the impacts of biomanufacturing on stakeholders with respect to associated benefits, risks, and consequences throughout its value chain. This implies taking actions that optimize positive social outcomes through adherence to ethical standards, including seeking ways to make products and processes that improve societal welfare. Attention to this commitment includes equitable distribution of benefits and risks and a responsiveness to society's needs and values.

Table 1: 4S Principles definitions as relevant to bioindustrial manufacturing

Significance/Impacts

The 4S principles: safety, security, sustainability, and social responsibility provide a useful framework for researchers, regulator, and companies seeking to build the bioeconomy

Attal-Juncqua et al., Trends in Biotechnology, /doi.org/10.1016/j.tibtech.2023.11.015