Conversion of biomass-derived carbohydrates to renewable N-heterocycles via spontaneous cascade reactions

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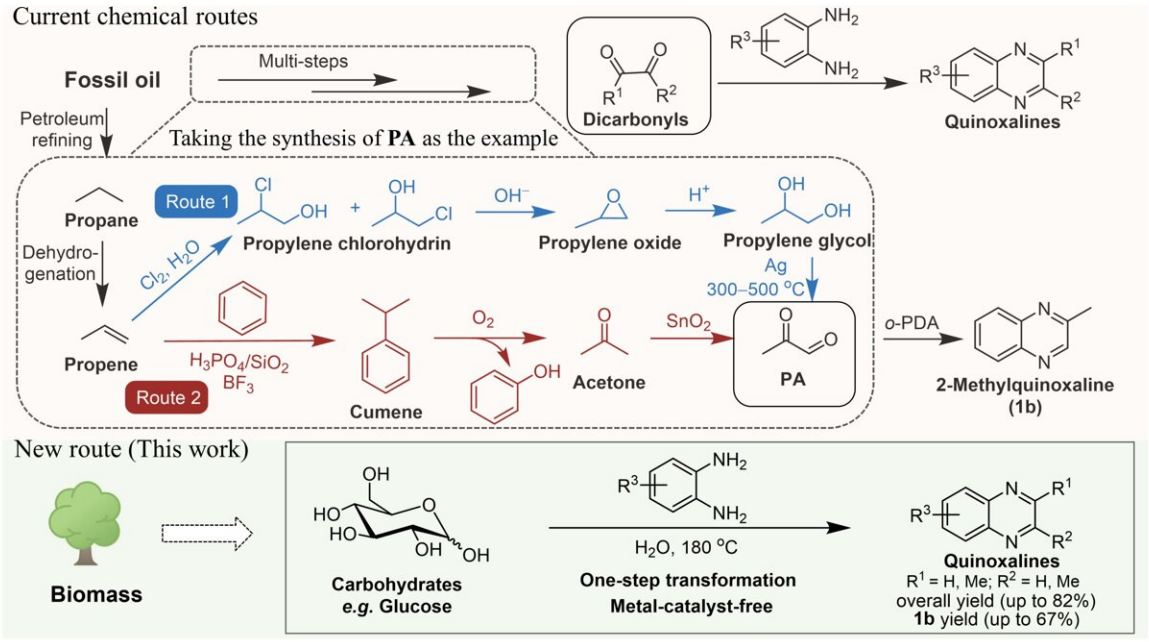

The upper part of the figure shows the current petroleum-based routes for manufacturing quinoxalines. The bottom part of the figure shows the proposed one-step sustainable approach based on biomass-derived carbohydrates. Credit: Science China Press

Research published in the journal *National Science Open* discloses a

novel synthetic approach for sustainable manufacturing of valuable quinoxalines, a type of N-heterocycle chemicals widely used in food, dye and pharmaceutical industries, directly from biomass-derived carbohydrates in presence of aryl-1,2-diamines, with the potential to replace currently cost-intensive petroleum-based synthetic routes as well as to accord with the future low-carbon footprint economy.

This one-step transformation could take place in water upon heating via spontaneous self-engineering of involved sequential cascade reactions even without using any eco-harmful metal catalysts/organic reagents and generate water as the solely theoretical byproduct, affording quinoxalines with up to 82 C% overall yield.

The reaction mechanism for this transformation is thoroughly studied by experiments and theory calculations. With this strategy, the standing challenging-to-overcome drawbacks related to the conventional fossil-based processes, such as the employment of environmentally hazardous metal catalysts/organic solvent/reagents, the required multistep transformations, and the resultant energy-intensive purification operations for each-step product, can be perfectly surmounted.

The authors further conceived integrated processes, which are compatible to current technology, for both batch and continuous-flow sustainable production of quinoxalines. Both integrated processes verified the robust and selective production of 2-methylquinoxalines, exhibiting excellent product yield and transformation stability even with recycling the aqueous reaction medium.

Furthermore, life-cycle assessment and techno-economic analysis of the proposed synthetic route were performed. The results indicate that both carbon footprint and production costs for manufacturing quinoxalines can be reduced significantly (by up to 30%) in contrast to the current fossil-based route. The environmental factor, a green chemistry metric,

of the process was estimated to be 0.4, much better than the conventional value (5-50) for fine chemicals production.

The study was led by Dr. Feng-Shou Xiao (College of Chemical and Biological Engineering, Zhejiang University) and Dr. Feng Yu (College of Chemical and Biological Engineering, Zhejiang University). The work was accomplished in collaboration with Fujian Institute of Research on the Structure of Matter (Dr. Chong Liu) and Guangzhou Institute of Energy Conversion (Dr. Yuping Li and Dr. Yuhe Liao), which belong to Chinese Academy of Sciences.

More information: Feng Yu et al, Sustainable production of value-added N-heterocycles from biomass-derived carbohydrates via spontaneous self-engineering, *National Science Open* (2023). DOI: 10.1360/nso/20230019

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