INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Investigations in Enhanced Production of Bioalcohols and Their Derivatives Using Experimental and in-Silico Approach

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SHORT ABSTRACT

This thesis presents a comprehensive scientific investigation focusing on the challenges and advancements in bioalcohol (mainly biobutanol) synthesis through *Clostridia*, emphasizing enhancing production efficiency from sustainable resources. Employing a multidisciplinary approach, the research encompasses comparative genomic analysis, in-depth exploration of cell central metabolism during ABE fermentation, experimental examination of butanol production from lignocellulosic hydrolysates using Clostridial co-culture systems, development of genome-scale metabolic models (GSMs), and innovative investigations into production of value-added bioalcohol using sono-enzymatic processes.

A key finding of the comparative genomic analysis is the successful identification of potential butanol-producing *Clostridium* species with an accuracy of 78%. This result provides insights into the genetic basis of bioalcohol production, providing a solid foundation for formulating potential engineering strategies to optimize biofuel synthesis.

The thesis has also analyzed physiological disparities between *C. acetobutylicum* and *C. pasteurianum* during ABE fermentation have been unveiled. Notably, *C. acetobutylicum* demonstrated superior performance with 25% higher growth rates and an impressive 18% increase in butanol production from various carbon sources. This understanding of coregulatory mechanisms and stress responses provided important inputs for strain optimization for enhanced bioalcohol production from sustainable sources.

The investigation into the inhibition mechanisms of key aldehyde/alcohol dehydrogenases (AADs) in solventogenic species led to the identification of ρ-coumaric acid (ρ-CA) as the most potent inhibitor. Its binding affinity to seven modeled enzymes highlights ρ-CA's significance as a potential target for enhanced biobutanol production, offering avenues for increased yields and cost-effectiveness.

Statistical optimization of Clostridial co-culture for bio-butanol production from mixed substrates resulted in exceptional yields of butanol (12.1 ± 0.45 g/L), biomass (4.15 ± 0.03 OD600), and ABE solvents (23.1 ± 0.55 g/L). The comprehensive Genome-scale models have given important insights in *Clostridium* ABE fermentation, the metabolic pathways, and potential targets for enhanced bioalcohol production.

The exploration of sonication-induced enhancement in lipase-catalyzed reactions for biodiesel synthesis, increased enzyme activity and faster reaction kinetics were observed. Structural modifications in lipases resulted in a higher yield of n-butyl levulinate (n-BL), opening promising avenues for efficient biodiesel production.

In conclusion, this thesis significantly contributes to the scientific understanding of Clostridial bioalcohol synthesis, offering vital knowledge for optimal strain selection, potential engineering strategies, and advancements in sustainable bioenergy production. Essentially, this dissertation has contributed to 3 among the 17 Sustainable Development Goals (SDGs) established by the United Nations in 2015, with the aim of achieving a more sustainable and inclusive future for all: (1) Goal 7 (affordable and clean energy), (2) Goal 11 (sustainable cities and communities), and (3) Goal 13 (climate action).