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Research Paper

Novel computational approach integrating genetic algorithms with multi-objective optimization to develop efficient protocols for analysing Cd, Pb, Cr and Hg in *Saccharum officinarum*

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ABSTRACT

Background: Heavy-metal contamination in sugarcane (Saccharum officinarum) can compromise food safety and requires extraction protocols that are both efficient and analytically defensible across chemically heterogeneous matrices (juice and lignocellulosic tissues).
Methods: A computational–experimental framework was developed that integrates sequential chemical extraction with ICP-OES quantification and a seven-objective NSGA-II optimizer to balance chemical performance (extraction efficiency, contamination resistance, and a phase-integrity/species-preservation proxy) against operational burden (time, reagent use, energy proxy, and cost). Experimental validation was conducted using n = 5 independent biological replicates per tissue type per condition, with replicate instrumental measurements and QA/QC gating (certified reference materials plus sugarcane matrix spikes) to ensure analytical accuracy and identify/retain only qualified batches. Agreement between computational predictions and experimental outcomes was evaluated using Bland–Altman limits-of-agreement and uncertainty propagation, while protocol performance differences were tested using Kruskal–Wallis omnibus tests followed by Benjamini–Hochberg–adjusted pairwise Mann–Whitney tests, with 95% bootstrap confidence intervals reported for key metrics (see SI Tables S4A–S4D; SI Fig. S11).
Results: Operational objectives exhibited rapid convergence, with 20–30% improvement by generation 15 relative to the initial population, followed by diminishing returns (SI Fig. S6–S9). Statistically significant differences among candidate protocols were observed for the primary objectives (omnibus tests $p < 0.05$; BH-adjusted pairwise comparisons reported in SI), and prediction–measurement agreement diagnostics supported the validity of experimentally qualified recommendations within the tested design space.
Significance: The framework provides a reproducible, uncertainty-aware pathway for optimizing sequential extraction protocols in complex sugarcane matrices while explicitly reporting replication, statistical support, and prediction–measurement agreement needed for defensible method development.

1. Introduction

Heavy metal contamination in food crops poses significant health and environmental risks worldwide [1], with sugarcane being particularly concerning due to its global importance as both a food source and biofuel feedstock [2]. Sugarcane (*Saccharum* spp.) cultivation spans over 26 million hectares across 90 countries, contributing approximately 80% of global sugar production [3] and 40% of biofuel needs [4]. The crop's economic significance extends beyond simple agricultural metrics, with the sugar industry supporting millions of livelihoods across

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