

Identification of Differential, Health-Related Compounds in Chardonnay Marc through Network-Based Meta-Analysis

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Objectives: Food/residue waste streams may be a significant source of bioactive compounds that benefit human health. Dietary intervention trials demonstrate the health benefits of such residues, but they are resource and time intensive. Bioinformatics meta-analyses can elucidate putative pathways, genes and chemicals that are relevant to human health, hence guiding further experimentation and intervention trials. To this end, we integrated publicly available phytochemical datasets related to general grape marc from different varieties (GM) and Chardonnay grape marc (CM) to investigate their differences and potential implications to human health through a network-based meta-analysis.

Methods: To characterize the phytochemical profile of grape marc, compositional data was aggregated from publicly available literature. To identify potential health effects based on this chemical information, associations between disease states and the chemical profiles of GM/CM

were extracted from the Comparative Toxicogenomics Database (CTD). Disease associative networks were constructed for a) marc products, b) all marc-related phenolics, c) compounds that are differentially abundant in CM.

Results: The union of available marc composition datasets from 14 articles contained 66 phenolic compounds; 29 of these were associated with at least 1 disease state in the CTD. There were 5 differentially over-abundant compounds in CM versus other grape marcs (red varieties $n = 75$, white varieties $n = 57$). These were flavan-3-ols catechin, epicatechin, epigallocatechin, galocatechin, and proanthocyanidin C1 ($P < 0.001$); with galocatechin unique to CM. Studies investigating marc products indicated associations to 15 diseases. CTD evidence from 934 studies associated the phenolic profile of GM to 358 diseases of 34 disease classes. Network-based meta-analysis suggested associations between GM and CM phenolics and several disease targets. This includes confirmatory associations between flavan-3-ols and cardiovascular disease outcomes.

Conclusions: Chardonnay marc is not widely studied; however, the developed framework of network-based meta-analysis utilizing composition information provides a holistic view of the knowledge space for grape marc, and highlights suggested health effects that can guide future research programs.

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