Metabolic profiling for benzoxazinoids in weed suppressive and early vigour wheat genotypes

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Summary Replicated and randomised wheat (*Triticum aestivum* L.) cultivar trials were conducted in moderate to low rainfall zones at Wagga Wagga (572 mm) and Condobolin (449 mm) NSW, respectively in 2014–2016. At each experimental site, crop and/or weed growth were monitored at selected growth stages including tillering, vegetative, grain filling, harvest and after crop harvest. In addition, shoots, roots, rhizoplane and bulk rhizosphere soil samples were collected for metabolomics profiling and biomass evaluation. Plant tissue samples were extracted in methanol using an automated Buchi high pressure extractor while soil samples were extracted using a rotary shaker. Extracts were filtered and specifically analysed for unique secondary metabolites or allelochemicals associated with weed suppression, specifically benzoxazinoids (BXs), using liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (UPLC-MS QToF). Metabolic profiling of wheat shoots, roots, and soils resulted in detection of up to 14 individual BXs including BX glycosides, lactones and hydroxamic acids of interest. Both qualitative and quantitative differences in BXs were observed and were cultivar-, growth stage- and location-dependent. Plant part and rhizosphere location (distance from root) also impacted BX concentration. Further metabolic profiling provided crucial information regarding crop metabolism, as well as the biosynthesis and release of metabolites associated with weed suppression in currently available commercial wheat cultivars, in contrast to weed suppressive rye (*Secale cereale* L.) and a heritage wheat cultivar Federation, both recognised for their potent ability to suppress weeds. We conclude that certain commercial wheat cultivars maintained high yield potential and were significantly more weed suppressive, depending on year and location, due to both their early growth habit and canopy architecture as well as the release of BX metabolites into the rhizosphere over time.

Keywords Weed suppression, metabolomics, residue, competition, resource allocation.