



Supplementary Figure S1. High resolution MS/MS spectra obtained in positive ionization of identified isomeric structures of sulphur-containing dicarboxylic acids whose presence in *Brachypodium* was suggested by pathway enrichment analysis. (A) 6'-methylthiohexylmalic acid; (B) 5'-methylthiopentylmalic acid. Main product ions and calculated chemical formulas have been indicated. Postulated structures with main fragmentation schemes are shown representatively as 2-(6'-methylthio)hexylmalic and 2-(5'-methylthio)pentylmalic acid, however, precise isomer identification requires further studies.