

## Description of Additional Supplementary Files

### **Supplementary Data 1. Summary of compound purification procedures and NMR analyses.**

Compound purification procedures and detailed NMR analyses are given for triticein, 3,5-dihydroxy-4',7-dimethoxyflavanone, 2'-*O*-demethyl triticein, and artocarpanone A.

### **Supplementary Data 2. Summary of variants in wheat TILLING lines used in this study.**

All variants are shown for wheat 'Cadenza' TILLING lines Cad1682, Cad1684, Cad1793, Cad0227, together with a sheet including only high impact variants of the four lines, and a sheet presenting only high impact variants found in relevant genes (cytochrome P450s and *O*-methyltransferases). SIFT score predicts whether an amino acid substitution is likely to affect protein function. Substitutions with a score < 0.05 are defined as deleterious.

### **Supplementary Data 3. Summary of BGC4(5D) Blastn analysis in wheat relatives.**

Blastn results used for construction of Figure 5b are shown separately for each species analyzed, including *T. aestivum* (subgenomes A/B), *T. turgidum ssp. dicoccoides*, *T. turgidum ssp. durum*, *A. tauschii*, *A. bicornis*, *A. longissima*, *A. speltoides*, *A. sharonensis*, *A. searsii*, *H. vulgare*, *B. distachyon*.