Figure S1. The optimal components of three PLSR models selected by one-sigma algorithm; a: the optimal components for pre-flowering PLSR model; b: the optimal components for post-flowering PLSR model; c: the optimal components for whole-stage PLSR model.
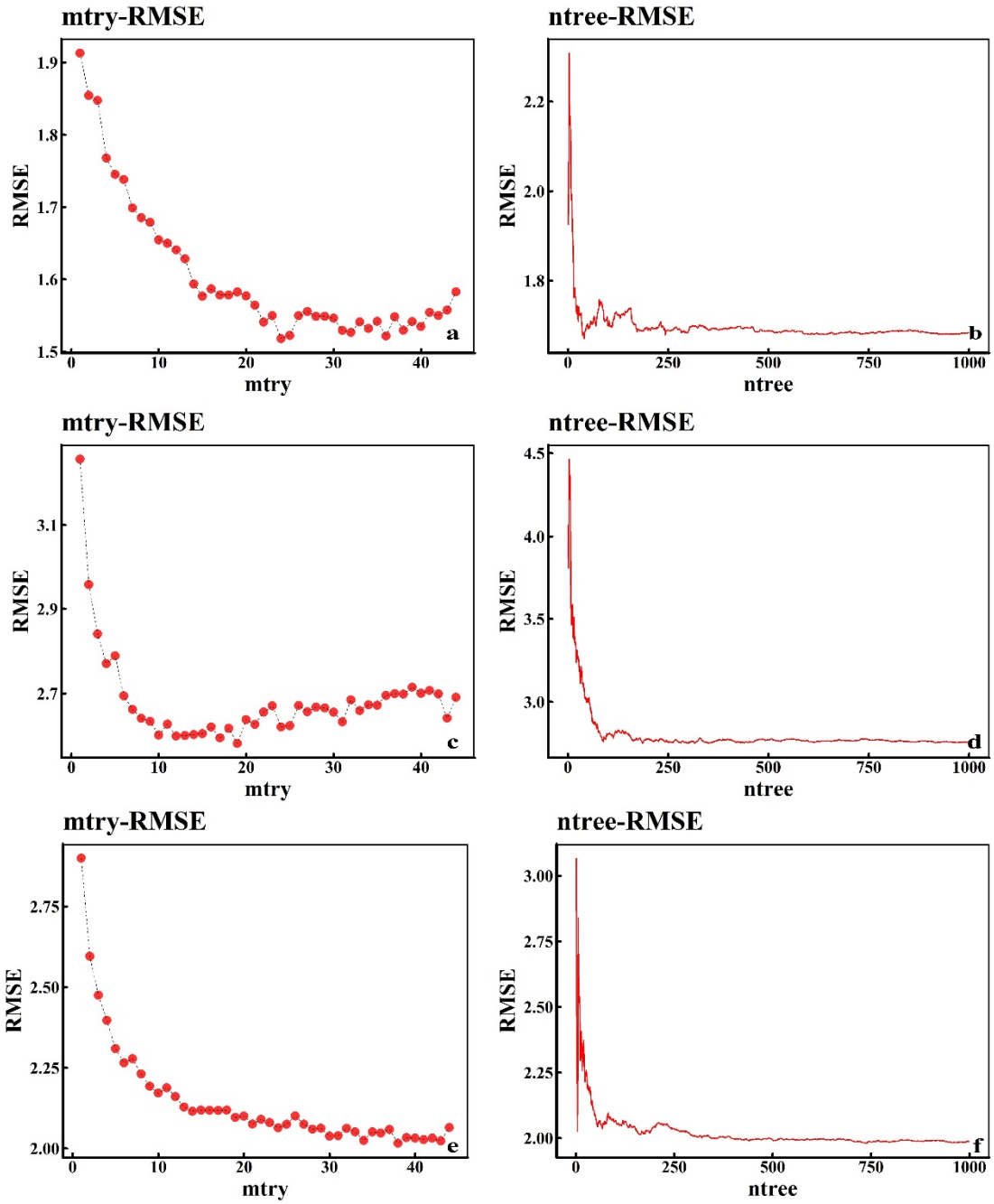
Figure S2. The *mtry* and *ntree* of three RF models; a-b: the *mtry* and *ntree* for pre-flowering RF model; c-d: the *mtry* and *ntree* for post-flowering RF model; e-f: the *mtry* and *ntree* for whole-stage RF model.
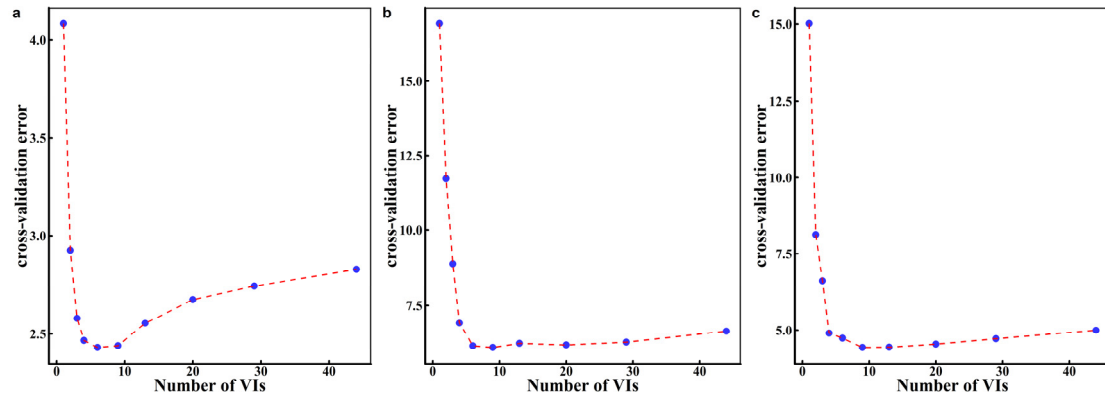
Figure S3. The cross-validation results of three RF models; a: the optimal *mtry* for pre-flowering RF model; b: the optimal *mtry* for post-flowering RF model; c: the optimal *mtry* for whole-stage RF model.