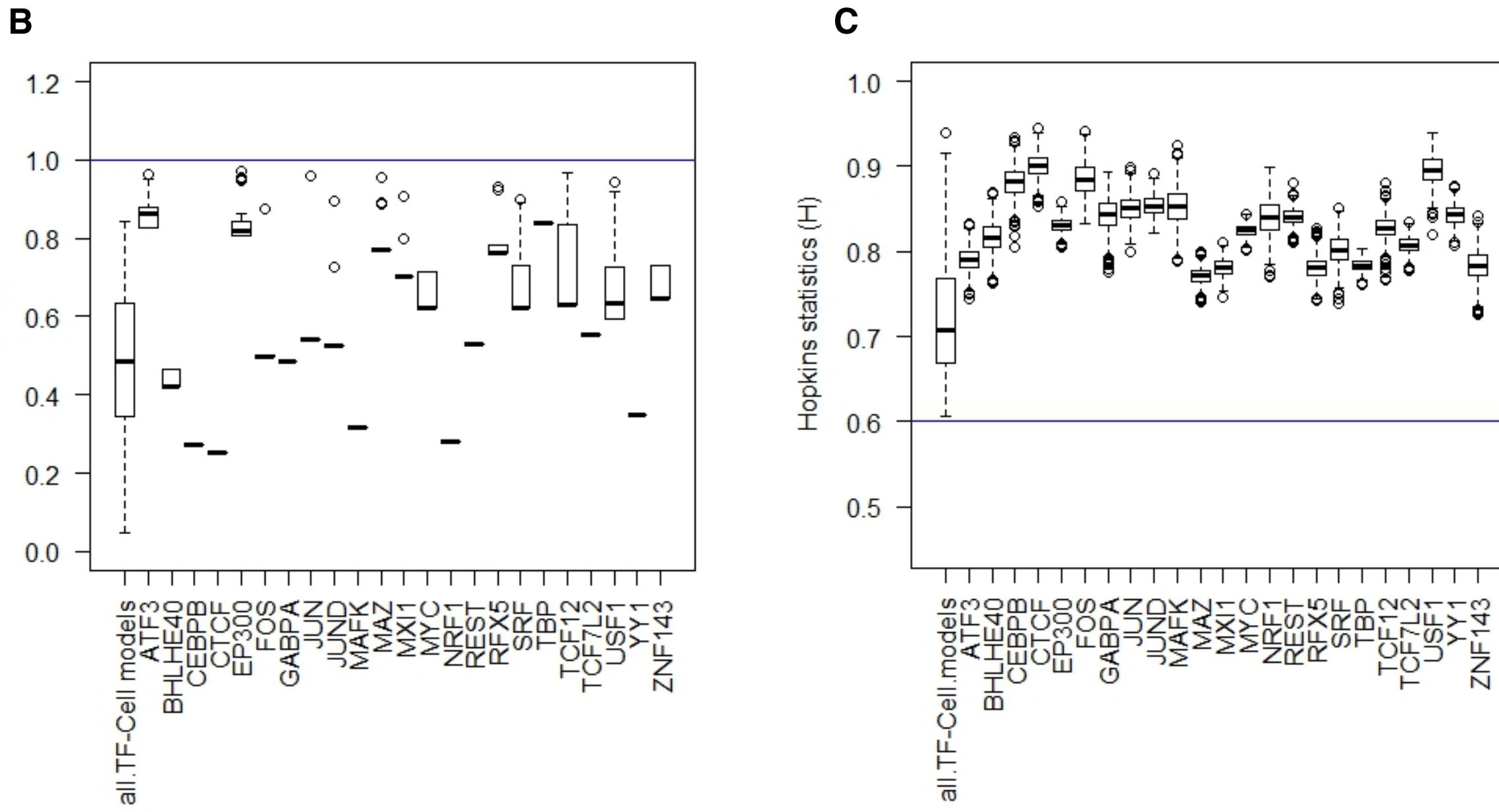
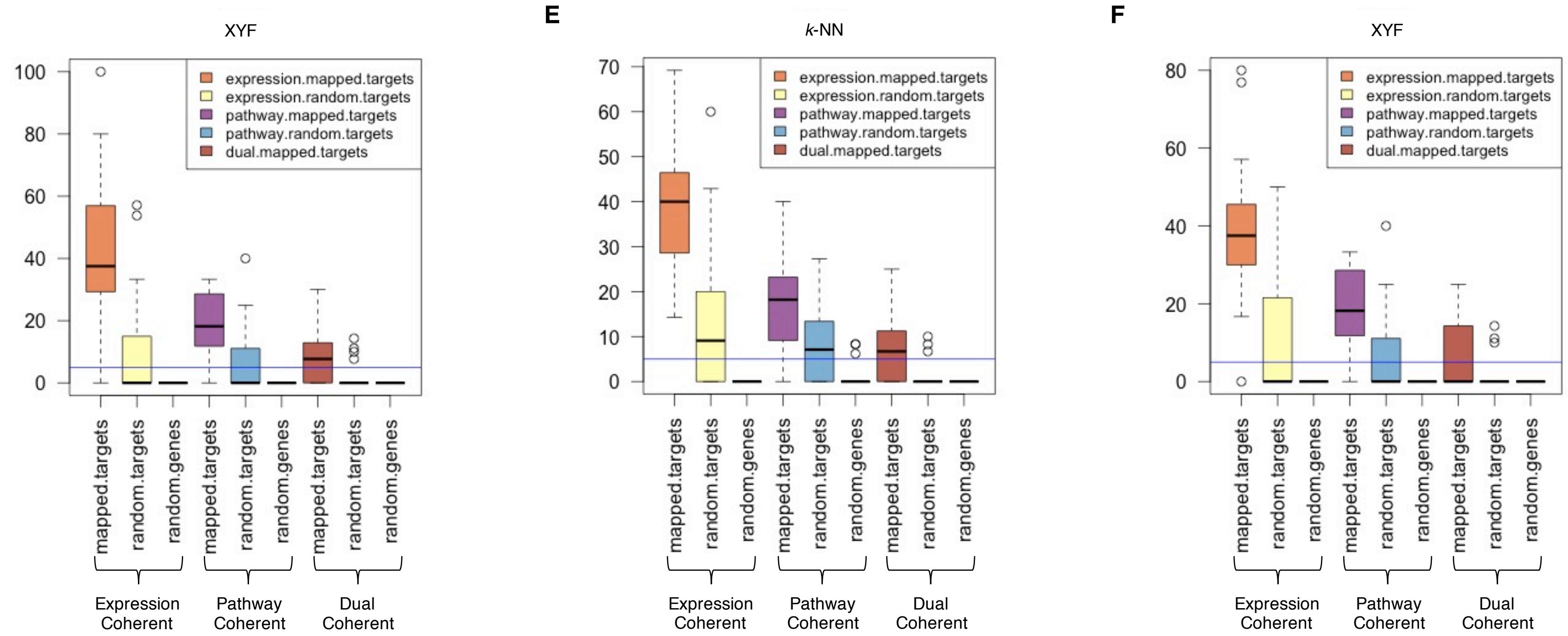


**Figure S6 (A).** Normalized within-cluster sum of squares stabilizes when the number of cluster is between 10 to 25; we choose  $k=16$  (denoted by the vertical line in the closer view) as a representative for all TFs.

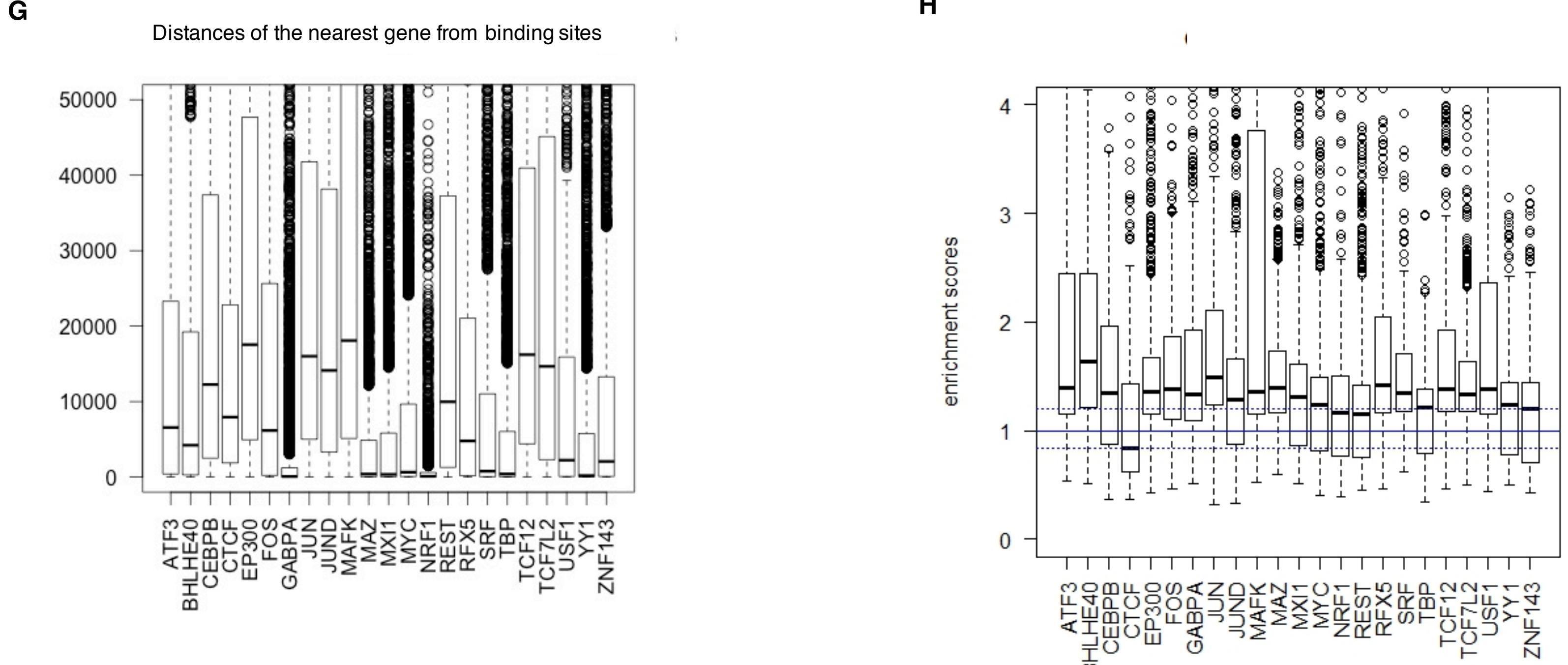


**Figure S6 (B-C).** Boxplot of *dh-ratio* (B), and *Hopkins statistic* (C) for 135 TF-cell pairs based on their sub-models, and pooled sub-models by TF. In (B), the horizontal line at  $Y=1$  denotes the maximum limit of *dh-ratio*. In (C), the horizontal line at  $Y=0.6$  denotes current lowest value of *Hopkins statistic*.



**Figure S6 (D).** Same plot as in Fig 2C, except the sub-models are clustered by XY-Fused (XYF) self-organizing map. In plot (D-F), the 'blue' horizontal line denotes the coherence in 5% of the total multi-clusters.

**Figure S6 (E-F).** Functional and Expression coherence of sub-model clusters with expression threshold of  $\log_{2}CPM \geq 5$ , i.e. a gene is considered as on when the  $\log_{2}CPM \geq 5$ . ~40% (~18%) multi-cell clusters show higher expression-coherence (pathway-coherence). Dual coherence denotes both expression and pathway coherence. (E) is drawn for *k*-NN (*k*-Nearest Neighbor) and (F) is drawn for XYF (XY fused network).



**Figure S6 (G).** Distance between binding sites and their nearest gene.

**Figure S6 (H).** Distribution of enrichment scores of all relevant co-factor motifs (with nonzero feature importance), for each TF separately. The horizontal line at  $Y=1$  denotes no enrichment/depletion, and the upper and lower dotted horizontal line denotes enrichment and depletion of 1.2 respectively.