

### **Description of Additional Supplementary Files**

**Supplementary Data 1.** Predicted drugs for breast cancer PDX model. P-values were determined by two-sided K-S test and were adjusted by BH FDR.

**Supplementary Data 2.** Predicted drugs for leukemia. P-values were determined by two-sided K-S test and were adjusted by BH FDR.

**Supplementary Data 3.** Predicted drugs for COVID-19. P-values were determined by two-sided K-S test and were adjusted by BH FDR.

**Supplementary Data 4.** FDA-approved drugs and compounds used in advanced clinical trials or have been proven effective in animal models