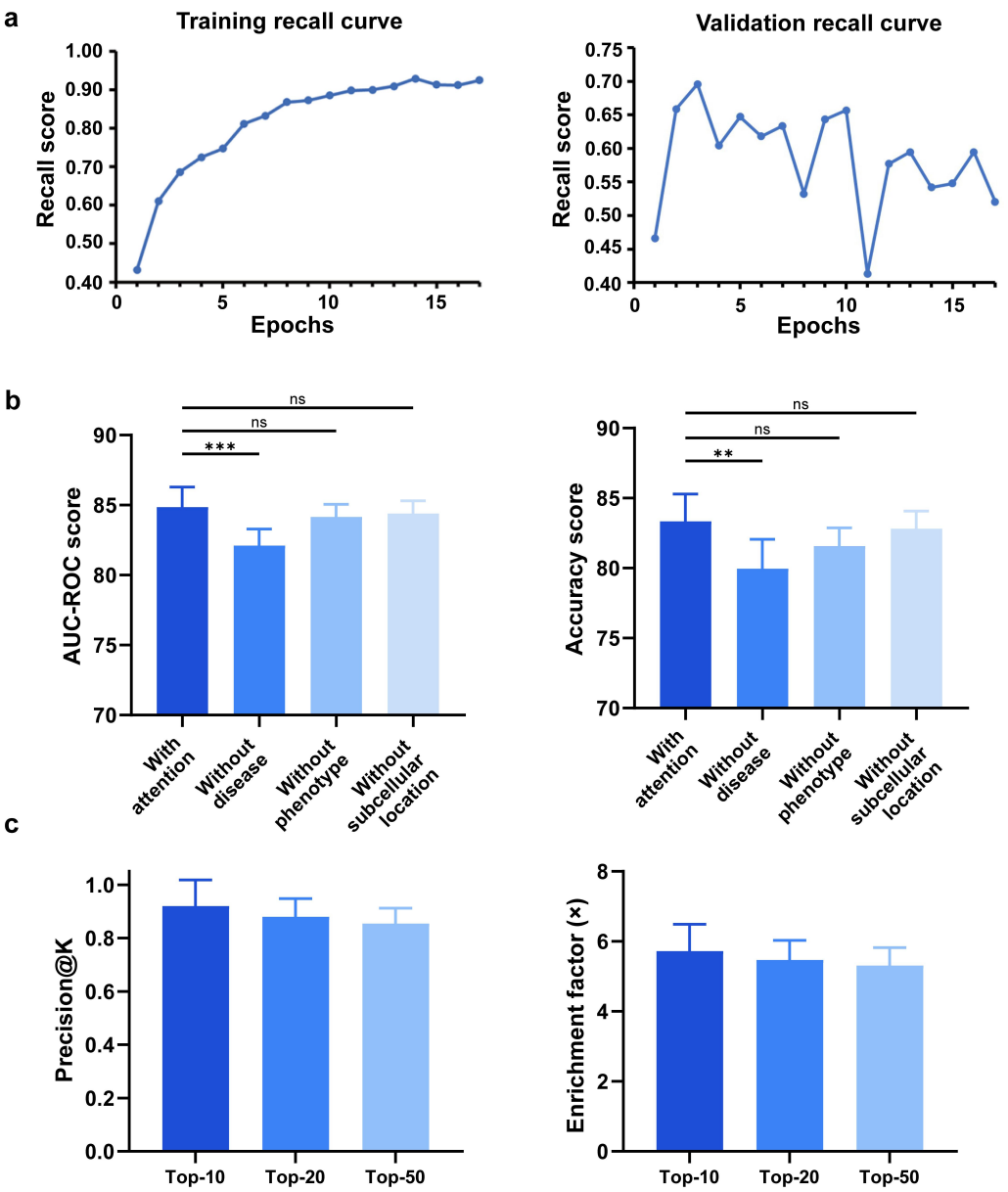

Figure S1. Performance evaluation of DeepETD. (a) Training and validation recall curves of the proposed model, showing model's capability to effectively identify positive samples. (b) Ablation study evaluating the contribution of different feature types to the model performance. The results indicate that disease association features contribute most to the predictive capability of DeepETD. ns, not significant, ** $P < 0.01$, *** $P < 0.001$; one-way ANOVA, data are presented as the mean ± SEM, $n = 5$. (c) Top-K prioritization performance evaluated by Precision@K and Enrichment Factor (×). The model maintained high precision and enrichment ability at lower K values, indicating effective prioritization of potential metabolite-target associations.