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Supplementary Note 1: Figure supplements

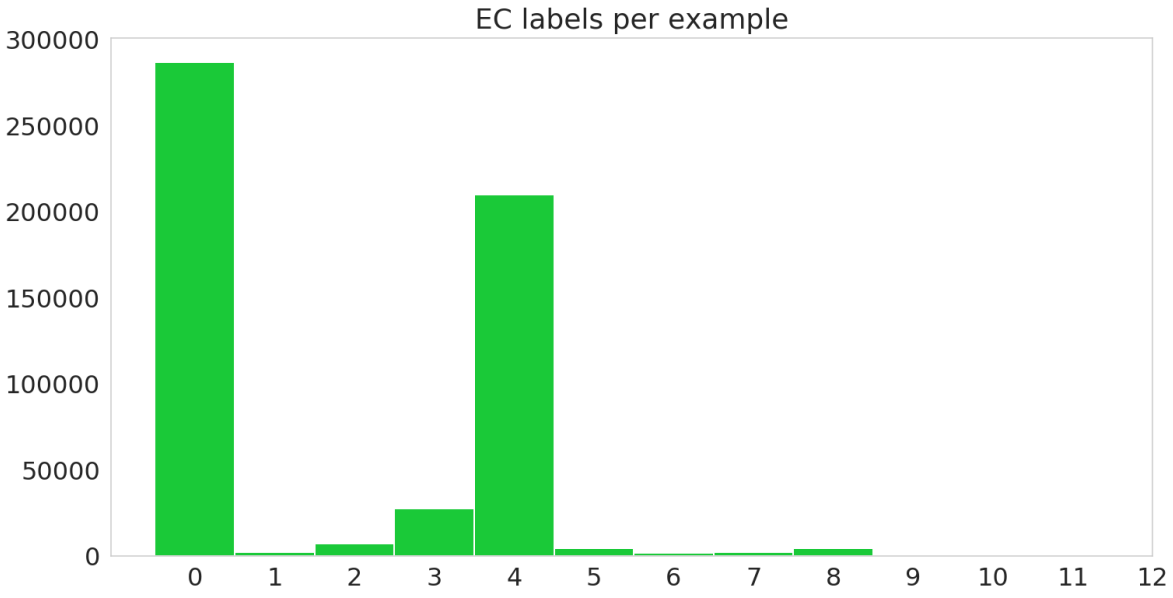


Fig. S1. [Figure 3 - Figure supplement 1] Histogram of number of labels per sequence, including hierarchical labels, on the random dataset.

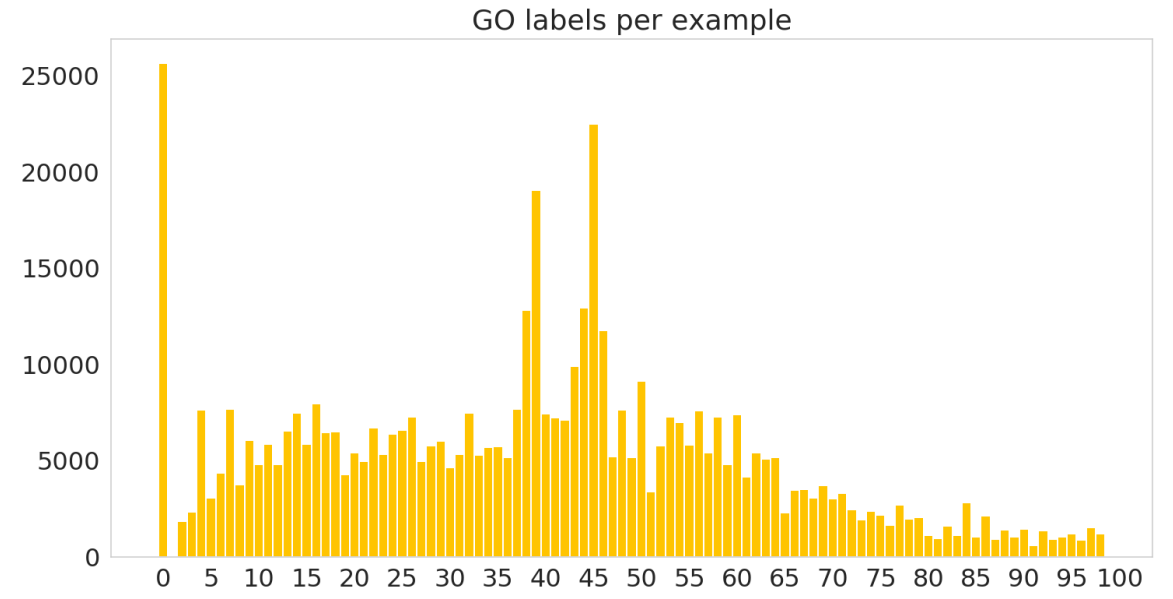


Fig. S2. [Figure 3 - figure supplement 2] Histogram of number of labels per sequence, including hierarchical labels, on the random dataset.

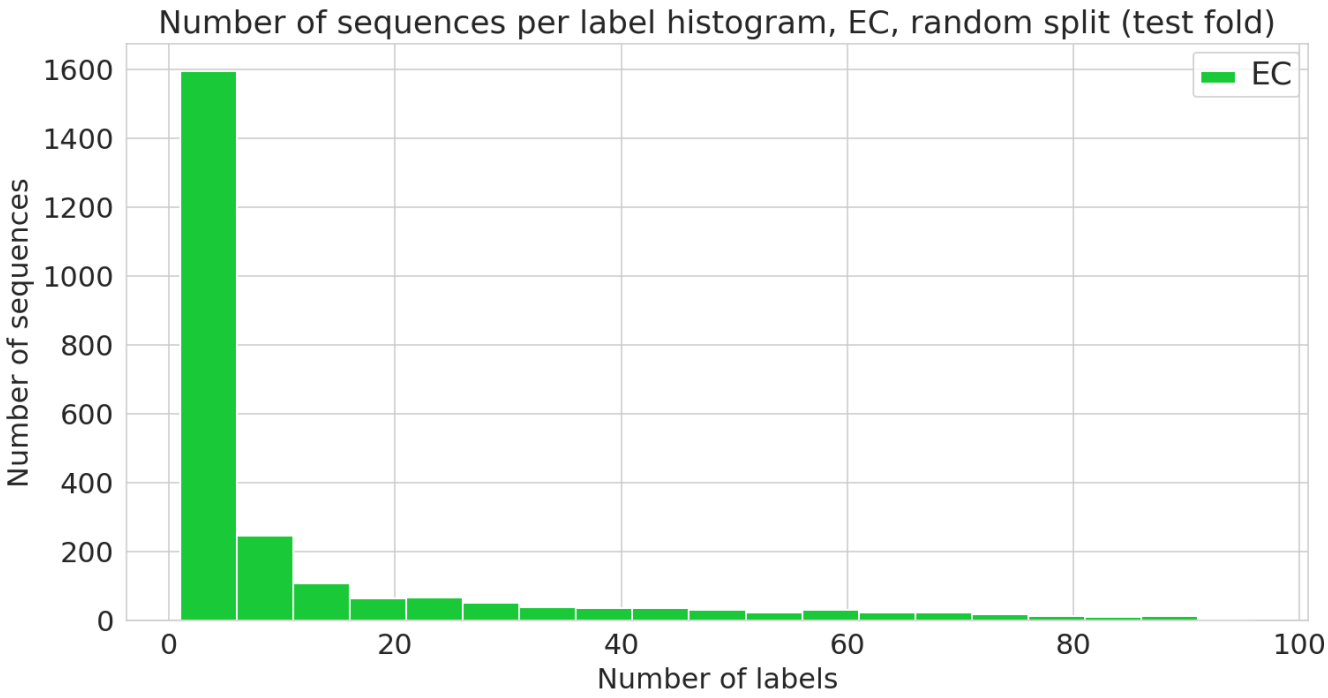


Fig. S3. [Figure 3 - figure supplement 3] Number of sequences annotated with a given functional label (EC class) in the random dataset.

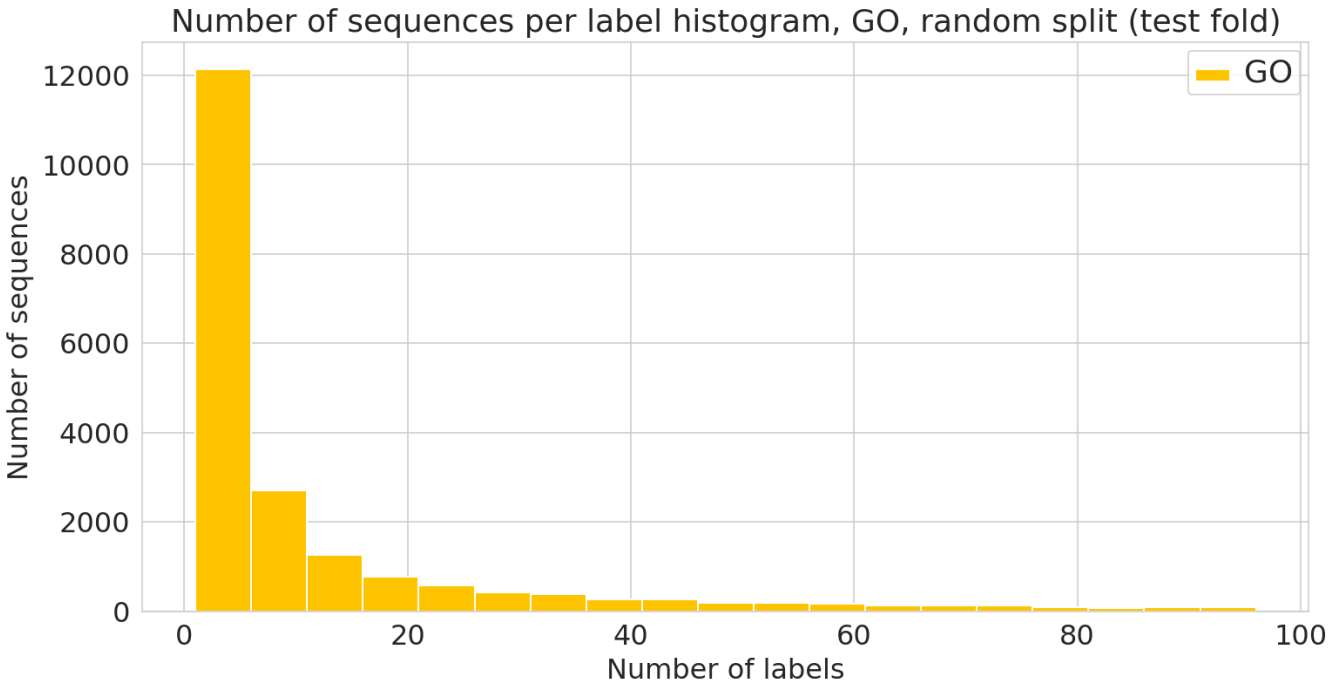


Fig. S4. [Figure 3 - figure supplement 4] Number of sequences annotated with a given functional label (GO label) in the random dataset.

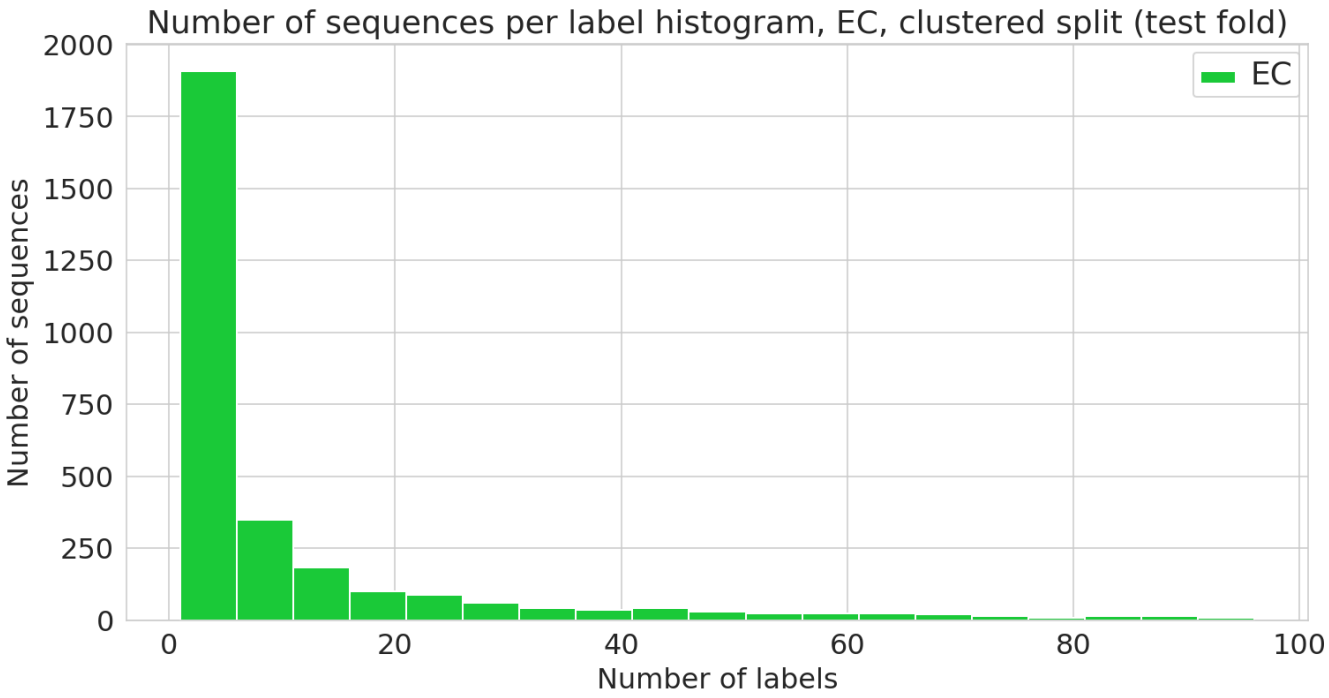


Fig. S5. [Figure 3 - figure supplement 5] Number of sequences annotated with a given functional label (EC class) in the clustered dataset.

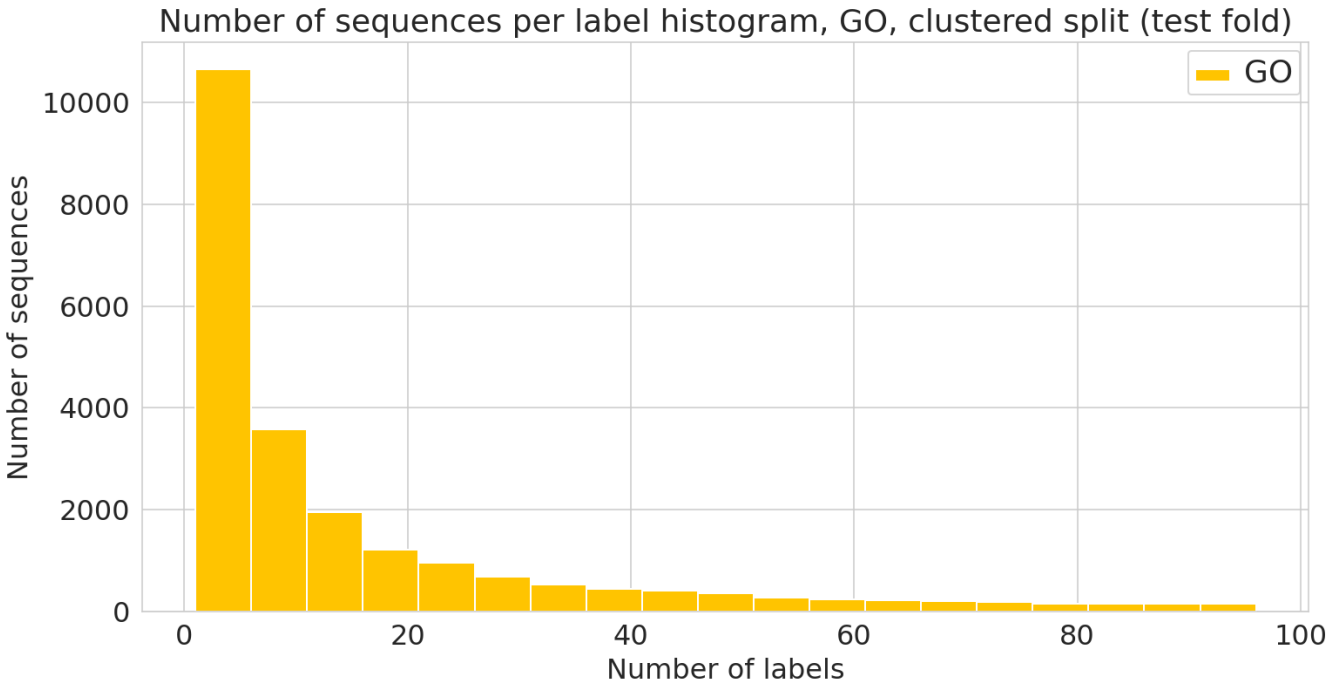
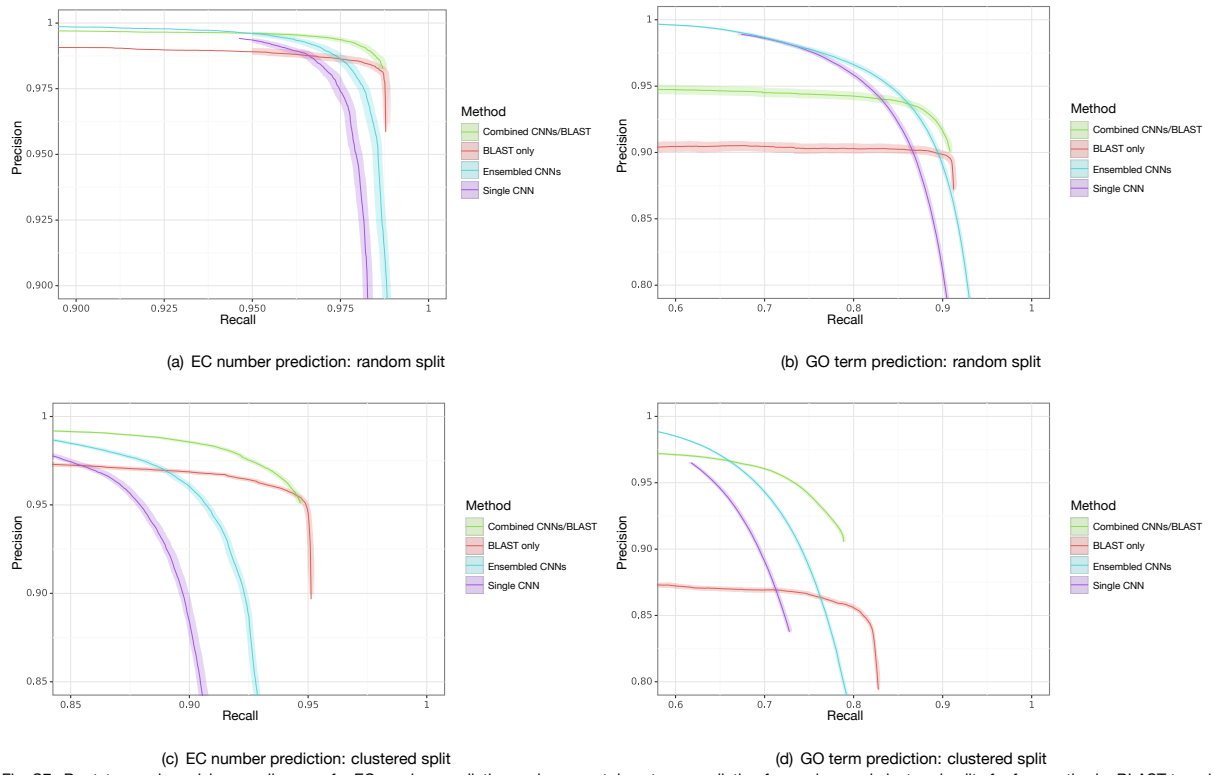


Fig. S6. [Figure 3 - figure supplement 6] Number of sequences annotated with a given functional label. (GO label) in the clustered dataset.



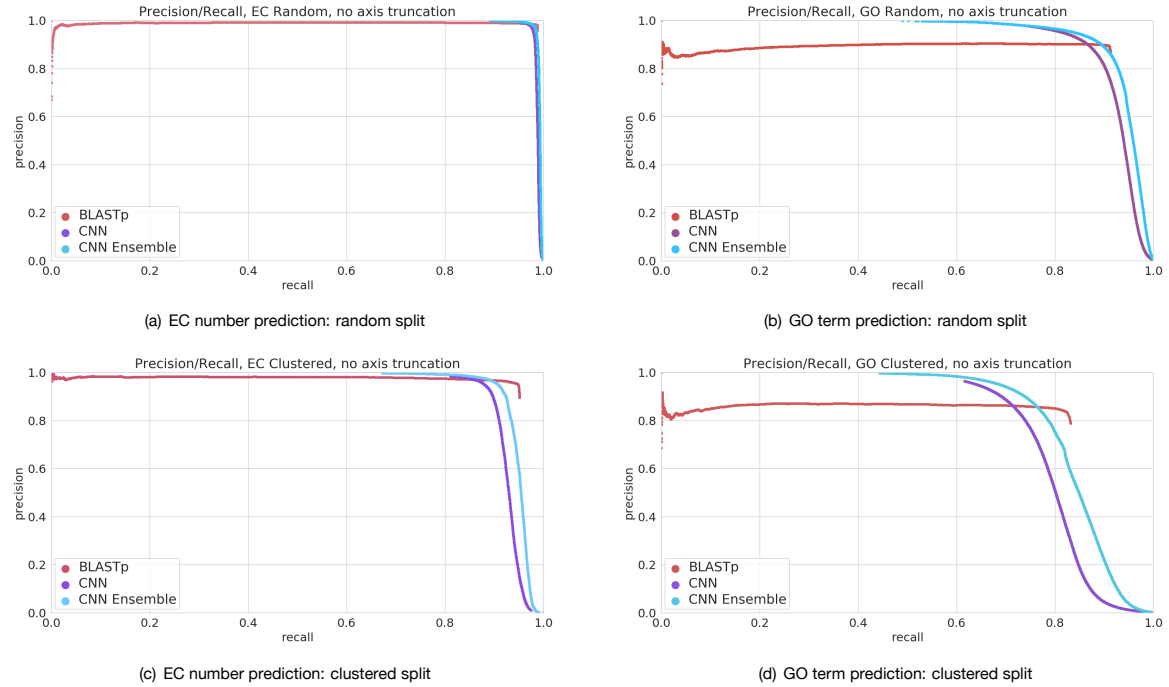
(a) EC number prediction: random split

(b) GO term prediction: random split

(c) EC number prediction: clustered split

(d) GO term prediction: clustered split

Fig. S7. [Figure 3 - figure supplement 7] Bootstrapped precision-recall curves for EC number prediction and gene ontology term prediction for random and clustered splits for four methods: BLAST top pick, single ProteInfer CNN, ensembled ProteInfer CNNs, and ensembled ProteInfer CNNs scaled by BLAST score.



(a) EC number prediction: random split

(b) GO term prediction: random split

(c) EC number prediction: clustered split

(d) GO term prediction: clustered split

Fig. S8. [Figure 3 - Figure supplement 8] Full precision-recall curves for EC number prediction and gene ontology term prediction for random and clustered splits for four methods: BLAST top pick, single ProteInfer CNN, ensembled ProteInfer CNNs

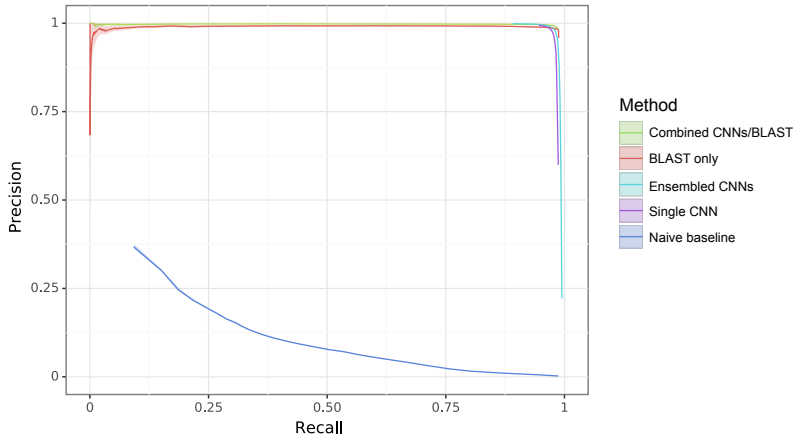


Fig. S9. [Figure 3 - Figure supplement 9] EC random task with different methods compared against a naive baseline where the predictor is simply the frequency in the training set.

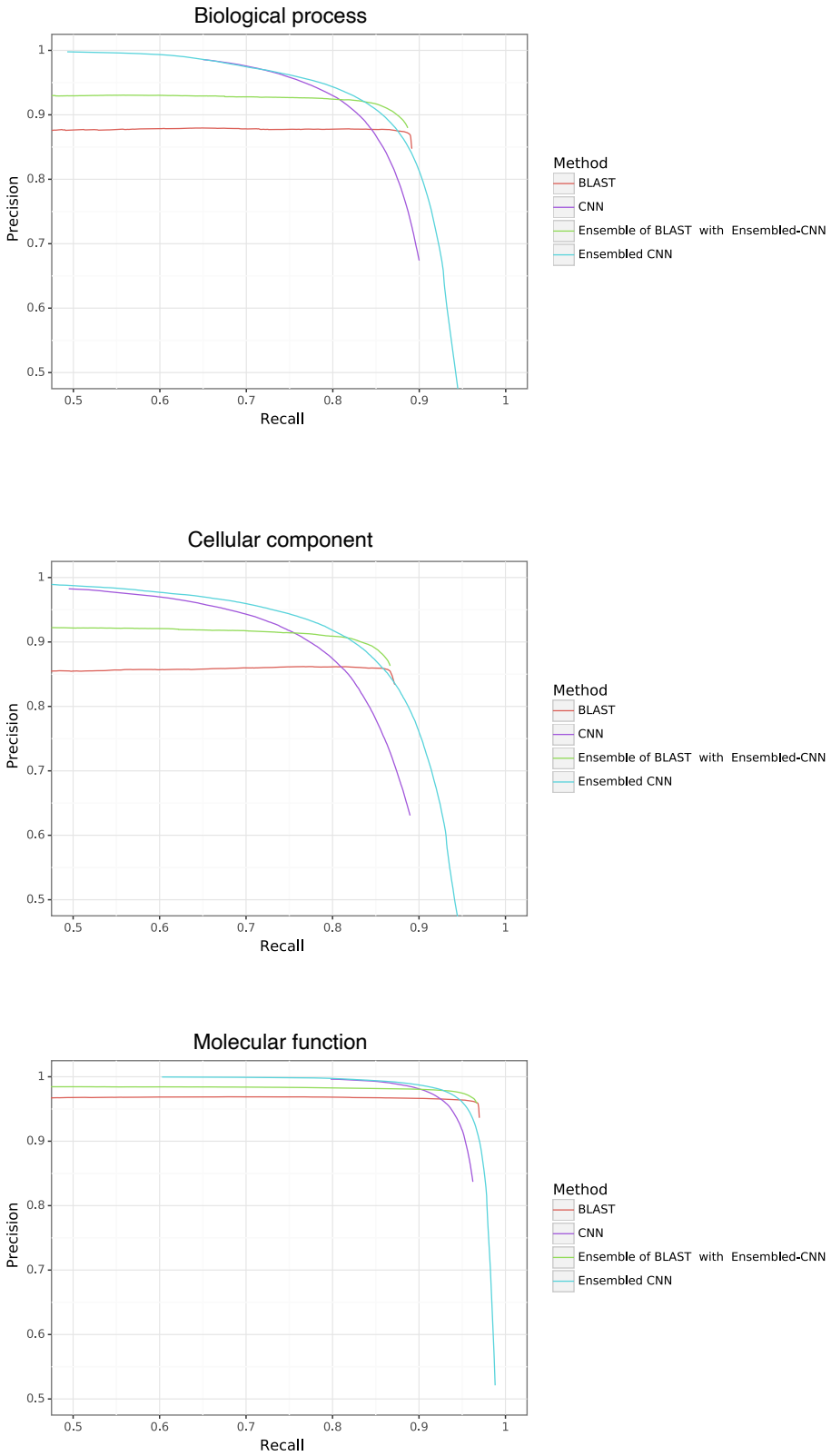


Fig. S10. [Figure 3 - Figure supplement 10] GO performance stratified by method and ontology type.

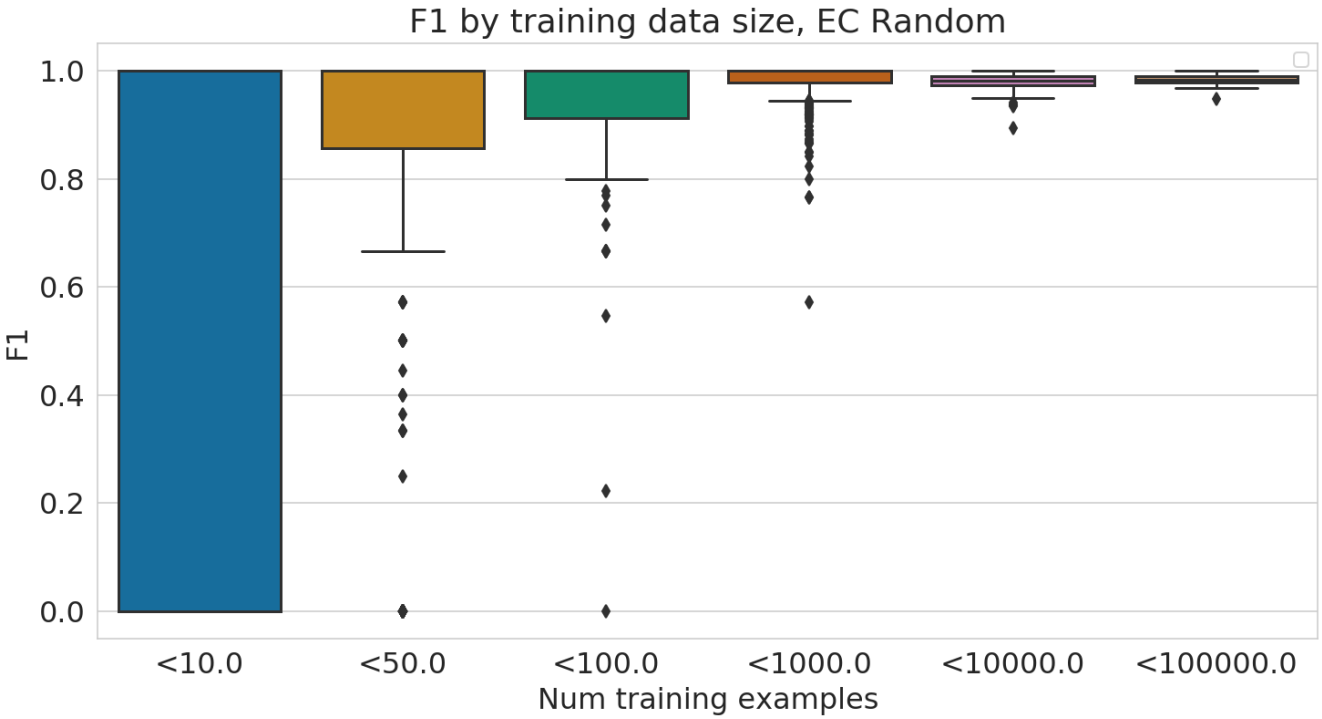


Fig. S11. [Figure 3 - Figure supplement 11] Performance of EC model stratified by number of training examples available for each test example.

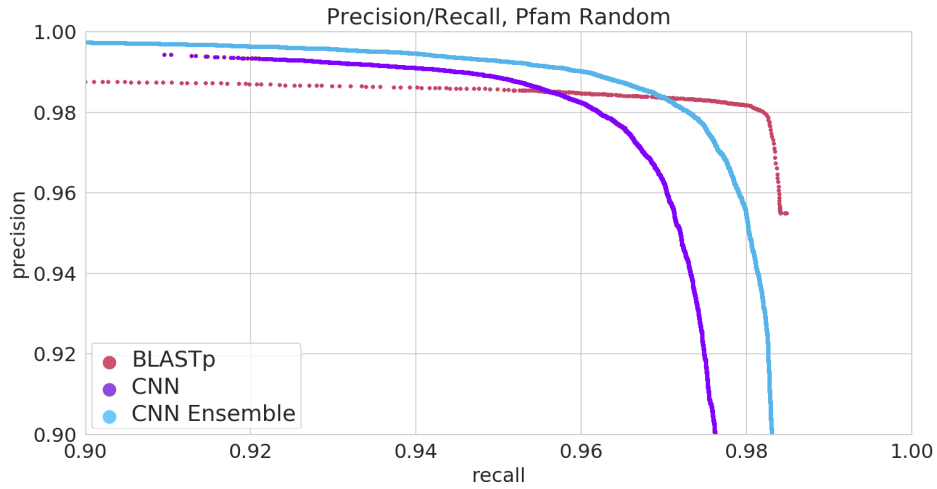


Fig. S12. [Figure 3 - Figure supplement 12] The ProteInfer algorithm is set up to allow any desired training vocabulary to be used. We demonstrated this by additionally training a model for predicting Pfam families from full-length protein sequences, which is available through our CLI-tool, and performs as shown here.