Table 1: The comparison results with pre-training methods ($\mathrm{F}_{\max}$) on GO term and EC number prediction. The best results are shown in bold.

Category	Method	GO-BP	GO-MF	GO-CC	EC
Sequence	ESM-1b [1]	0.452	0.659	0.477	0.869
	ESM-2 [2]	0.454	0.624	0.545	0.874
Sequence-Function	ProtST-ESM-1b [3]	0.480	0.661	0.488	0.878
	ProtST-ESM-2 [3]	0.482	0.668	0.487	0.878
Sequence-Structure	ESM-S [4]	0.463	0.649	**0.519**	0.823
	ESM-GearNet [5]	0.516	0.684	0.506	0.890
	SaProt [6]	0.356	0.678	0.414	0.884
	ESM-CoupleNet (Ours)	**0.521**	**0.688**	0.516	**0.894**

Table 2: Experimental results comparison on the CATH dataset (inverse folding).

Model	Perplexity ↑			Recovery (%) ↓		
	Short	Single	All	Short	Single	All
ESM-IF [7]	8.18	6.33	6.44	31.30	38.50	38.30
PiFold [8]	6.04	6.31	4.55	39.84	38.53	51.66
VFN-IF [9]	5.70	5.86	4.17	41.34	40.98	**54.74**
CoupleNet (Ours)	**5.68**	**5.74**	**4.04**	**41.92**	**41.63**	54.34

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