

Table S4: Downstream results for the ablations not included in the main text on the datasets from [17]. The tasks comprise ThermoStability (regression) evaluated using Spearman correlation, HumanPPI, Metal Ion Binding, DeepLoc Binary (binary classification) and DeepLoc Subcellular (multiclass classification), evaluated using accuracy (ACC) and Area Under the Receiver Operating Curve (AUC), Enzyme Commission numbers (EC), Gene Ontology (GO) terms corresponding to Molecular Function (MF), Biological Process (BP) and Cellular Component (CC) evaluated using maximum F1-score metric (Fmax) defined by formula (6) of the main text. ST corresponds to Structure Token modality, SG corresponds to Structure Graph modality, '+' indicates a combination of multiple modalities.

Model	Thermostability	HumanPPI	Metal Ion Binding	EC	GO			DeepLoc	
	Spearman's $\rho$	ACC%	ACC%	Fmax	MF Fmax	BP Fmax	CC Fmax	Subcellular ACC%	Binary ACC%
<b>Pocket</b>	0.601 (0.022)	75.8/84.8 (1.1/1.2)	66.1/70.8 (1.4/1.5)	0.843 (0.003)	0.604 (0.027)	0.437 (0.003)	0.473 (0.003)	62.1 (0.9)	83.6 (0.6)
<b>Text+Pocket</b>	<b>0.670</b> (0.008)	<b>86.1/93.7</b> (1.6/0.7)	72.6/83.0 (0.9/0.7)	0.872 (0.004)	<b>0.659</b> (0.003)	0.497 (0.003)	0.547 (0.006)	<b>81.5</b> (0.4)	<b>92.3/96.5</b> (0.2/0.1)
<b>SG</b>	0.616 (0.011)	77.3/84.2 (1.6/1.2)	63.9/72.3 (1.6/1.9)	0.698 (0.004)	0.467 (0.004)	0.367 (0.003)	0.447 (0.011)	62.0 (0.7)	82.8/89.5 (0.7/0.7)
<b>SG+Pocket</b>	0.616 (0.011)	81.2/87.2 (1.1/0.9)	68.2/70.8 (2.0/0.9)	0.829 (0.001)	0.589 (0.005)	0.425 (0.003)	0.473 (0.003)	63.0 (0.3)	84.0/90.4 (0.6/0.4)
<b>ST</b>	0.623 (0.018)	79.1/89.0 (1.7/0.6)	67.6/78.2 (2.5/0.4)	0.863 (0.003)	0.630 (0.005)	0.459 (0.003)	0.497 (0.011)	66.9 (0.7)	86.8/92.8 (0.4/0.2)
<b>ST+Pocket</b>	0.633 (0.016)	78.2/83.8 (2.5/1.1)	65.9/73.6 (2.0/1.2)	0.865 (0.003)	0.637 (0.004)	0.461 (0.003)	0.501 (0.009)	65.2 (0.7)	87.6/92.1 (0.5/0.3)
<b>ST+SG</b>	0.636 (0.006)	85.3/90.9 (1.4/1.8)	68.6/74.8 (0.8/2.1)	0.850 (0.003)	0.609 (0.026)	0.448 (0.002)	0.503 (0.008)	68.1 (0.7)	89.2/94.2 (0.4/0.2)
<b>ST+SG+Text</b>	0.669 (0.006)	85.0/93.1 (1.1/0.6)	<b>74.6/83.2</b> (0.3/1.2)	<b>0.875</b> (0.002)	0.654 (0.004)	0.493 (0.002)	<b>0.549</b> (0.003)	80.9 (0.4)	92.1/93.1 (0.2/0.2)
<b>ST+SG+Pocket</b>	0.642 (0.005)	77.3/85.6 (1.9/1.7)	65.5/71.8 (2.7/1.5)	0.861 (0.005)	0.627 (0.003)	0.459 (0.003)	0.498 (0.008)	66.2 (0.5)	87.9/93.1 (0.5/0.5)
<b>OneProt-4 matched</b>	0.647 (0.011)	85.7/94.5 (0.9/0.3)	74.3/81.8 (1.5/0.9)	0.867 (0.004)	0.651 (0.003)	0.491 (0.002)	0.549 (0.008)	80.8 (0.4)	91.9/96.3 (0.4/0.1)