Applying the CLEAN Model to MUTarget Data

Loss Function	Selection Method	Validation Fold	Validation Precision	Validation Recall	Validation F1	Validation AUC	Test Fold	Test Precision	Test Recall	Test F1	Test AUC
		0	0.809	0.853	0.818	0.912	1	0.796	0.879	0.825	0.92
		1	0.783	0.865	0.809	0.916	2	0.772	0.835	0.79	0.898
Triplet	MaxSep	2	0.798	0.846	0.808	0.903	3	0.821	0.88	0.836	0.929
		3	0.821	0.856	0.821	0.917	4	0.805	0.827	0.8	0.898
		4	0.813	0.86	0.822	0.914	0	0.813	0.855	0.819	0.915
			0.8048	**0.856**	**0.8156**	**0.9124**		**0.8014**	**0.8552**	**0.814**	**0.912**
		0	0.845	0.783	0.805	0.878	1	0.827	0.794	0.808	0.875
		1	0.821	0.778	0.793	0.875	2	0.829	0.753	0.782	0.859
Triplet	Pvalue	2	0.84	0.741	0.777	0.85	3	0.856	0.774	0.806	0.876
		3	0.845	0.736	0.774	0.856	4	0.821	0.699	0.744	0.836
		4	0.837	0.746	0.782	0.857	0	0.843	0.753	0.786	0.865
			0.8376	**0.7568**	**0.7862**	**0.8632**		**0.8352**	**0.7546**	**0.7852**	**0.8622**
		0	0.819	0.853	0.828	0.915	1	0.82	0.853	0.83	0.916
		1	0.782	0.849	0.807	0.909	2	0.797	0.831	0.806	0.892
SupCon	MaxSep	2	0.814	0.825	0.81	0.893	3	0.856	0.872	0.852	0.925
		3	0.821	0.845	0.818	0.911	4	0.814	0.853	0.823	0.91
		4	0.82	0.855	0.829	0.913	0	0.83	0.84	0.823	0.908
			0.8112	**0.8454**	**0.8184**	**0.9082**		**0.8234**	**0.8498**	**0.8268**	**0.9102**
		0	0.843	0.819	0.827	0.898	1	0.839	0.822	0.827	0.9
		1	0.847	0.825	0.834	0.9	2	0.827	0.782	0.8	0.868
SupCon	Pvalue	2	0.842	0.783	0.806	0.87	3	0.867	0.836	0.847	0.907
		3	0.851	0.791	0.812	0.884	4	0.838	0.797	0.809	0.881
		4	0.847	0.818	0.827	0.895	0	0.854	0.809	0.823	0.893
			0.846	**0.8072**	**0.8212**	**0.8894**		**0.845**	**0.8092**	**0.8212**	**0.8898**

① 'dual' is included by mistake
② Triplet model trained for 2500 epochs
③ SupCon model trained for 1500 epochs, n_pos = 9, n_neg = 30, T = 0.1
④ In the P-value method, P = 1e-5, nk_random = 20k