

Table 1: % of bootstraps where a given embedding method yielded better model performance than the baseline

	Unseen treatment	One-hot encoding	SMILES-based embeddings	K
0	adalimumab	0.00%	0.00%	30
1	azathioprine	40.00%	0.00%	20
2	balsalazide	10.00%	90.00%	0.5
3	cyclosporine	0.00%	20.00%	40
4	golimumab	10.00%	0.00%	80
5	infliximab	100.00%	0.00%	30
6	mercaptopurine	70.00%	0.00%	40
7	mesalazine	10.00%	20.00%	20
8	olsalazine	60.00%	20.00%	30
9	sulfasalazine	50.00%	100.00%	0.5
10	tacrolimus	30.00%	70.00%	10
11	tofacitinib	50.00%	70.00%	90
12	ustekinumab	0.00%	0.00%	0.5
13	vedolizumab	0.00%	0.00%	60