Table S1. The specific hyper-parameter settings on baseline methods

Baseline	Dropout	Learning_rate	Batch_size	optimizer	Activation
CNN_FP2	0.4	1e-3	64	Adam	RELU
BERT_smiles	0.4	1e-4	64	Adam	RELU
Attentive_FP	0.4	1e-3	64	Adam	RELU