		Method		
Test Set	Performance	QUBO-based Maximum	QUBO-based Maximum	MACCS
	Metric	Weighted Co-3-plex	Weighted Co-1-plex	Fingerprint
Set 1	Accuracy	0.81	0.80	0.76
	Precision	0.79	0.77	0.69
	Sensitivity	0.84	0.85	0.95
	Specificity	0.78	0.75	0.58
Set 2	Accuracy	0.80	0.79	0.77
	Precision	0.78	0.77	0.70
	Sensitivity	0.83	0.85	0.95
	Specificity	0.77	0.74	0.60