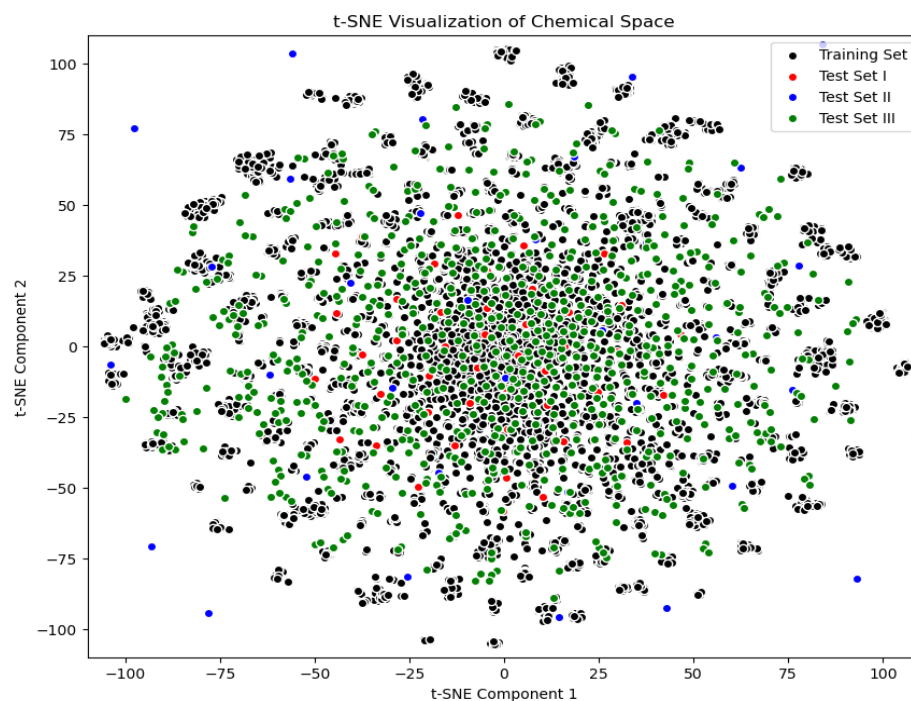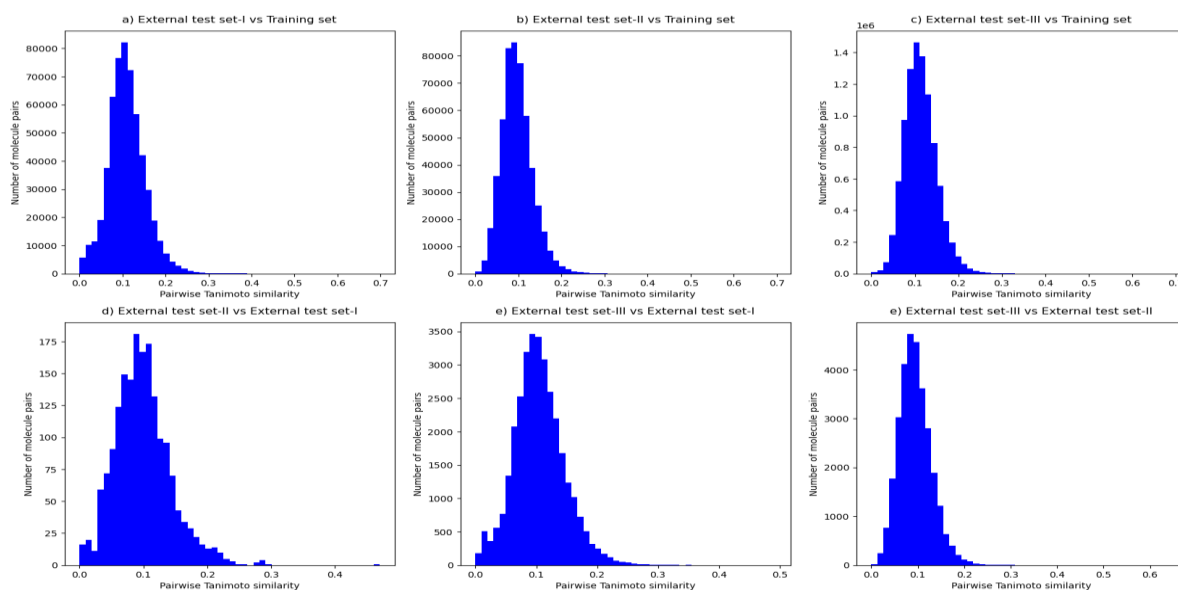## Replicated Metrics

A table replicating the metric value on the three test dataset used in the publication

Evaluation data	Method	MCC	NPV	ACC	PPV	SPE	SEN	B-ACC
Test set-I	Cardiotox	0.599	0.688	0.81	0.893	0.786	0.833	0.81
Test set-II	Cardiotox	0.452	0.947	0.755	0.455	0.6	0.909	0.755
Test set-III	Cardiotox	0.22	0.986	0.746	0.112	0.698	0.794	0.746

t-SNE Visualization of Chemical Space

Replicated Taniomoto similarity graph

a) External test set-I vs Training set   b) External test set-II vs Training set   c) External test set-III vs Training set

d) External test set-II vs External test set-I   e) External test set-III vs External test set-I   e) External test set-III vs External test set-II

Output Metric for test set I using model in Ersilia hub

Evaluation data	Method	MCC	NPV	ACC	PPV	SPE	SEN	B-ACC
Test set-I	Cardiotox	0.599	0.688	0.81	0.893	0.786	0.833	0.81