

Table B. Aggregated results of cross-validation, using TICF; without the relational network.

ML Model	Train R2		Explained Variance		Negative Mean Absolute Error		Negative Median Absolute Error	
	Mean	StD	Mean	StD	Mean	StD	Mean	StD
SVR-RBF	0.119	0.171	0.283	0.041	-35.024	3.852	-31.768	8.111
SVR-LINEAR	0.876	0.024	0.896	0.015	-13.733	2.758	-12.726	2.579
DTR	0.984	0.011	0.988	0.006	-4.727	1.760	-4.449	1.709
SVR-POLY	0.006	1.845	0.102	1.708	-21.943	13.774	-14.637	4.944