

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R ² ↑
eqV2	0.896	5.243	0.900	0.965	0.893	0.979	0.020	0.071	0.842
ORB	0.858	5.281	0.906	0.954	0.815	0.983	0.028	0.078	0.814
MatterSim	0.832	4.838	0.830	0.942	0.834	0.965	0.026	0.079	0.809
GNoME	0.810	4.810	0.825	0.942	0.796	0.965	0.034	0.083	0.786
eqV2 DeNS	0.798	4.362	0.748	0.927	0.855	0.941	0.035	0.084	0.785
ORB MPtrj	0.755	4.188	0.719	0.911	0.795	0.936	0.043	0.090	0.752
SevenNet	0.719	3.804	0.653	0.893	0.800	0.912	0.046	0.090	0.750
MACE	0.668	3.400	0.583	0.867	0.781	0.885	0.055	0.099	0.698
CHGNet	0.612	3.038	0.521	0.839	0.740	0.859	0.061	0.100	0.690
M3GNet	0.576	2.647	0.454	0.802	0.788	0.804	0.072	0.115	0.588
ALIGNN	0.565	2.921	0.501	0.829	0.649	0.866	0.092	0.154	0.274
MEGNet	0.513	2.699	0.463	0.813	0.574	0.862	0.128	0.204	-0.277
CGCNN+P	0.510	2.398	0.411	0.779	0.670	0.801	0.108	0.178	0.027
CGCNN	0.510	2.631	0.451	0.807	0.587	0.852	0.135	0.229	-0.624
Wrenformer	0.479	2.130	0.365	0.741	0.693	0.751	0.105	0.182	-0.020
BOWSR	0.437	1.836	0.315	0.702	0.711	0.680	0.114	0.164	0.142
Voronoi RF	0.344	1.509	0.259	0.665	0.511	0.697	0.141	0.206	-0.316
Dummy	0.194	1	0.168	0.680	0.231	0.770	0.120	0.181	0