

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R ² ↑
eqV2 S DeNS	0.798	4.362	0.748	0.927	0.855	0.941	0.035	0.084	0.785
AlphaNet-MPTrj	0.789	4.312	0.740	0.923	0.846	0.938	0.040	0.091	0.747
DPA3-v1-MPtrj	0.757	4.130	0.709	0.911	0.812	0.931	0.040	0.082	0.793
ORB MPtrj	0.755	4.188	0.719	0.911	0.795	0.936	0.043	0.090	0.752
SevenNet-l3i5	0.751	4.112	0.706	0.909	0.803	0.931	0.042	0.086	0.773
SevenNet-0	0.719	3.804	0.653	0.893	0.800	0.912	0.046	0.090	0.750
GRACE-2L-MPtrj	0.687	3.714	0.637	0.884	0.746	0.912	0.050	0.092	0.740
MACE-MP-0	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	1.000	0.168	0.680	0.231	0.770	0.120	0.181	0.000