

Supplementary Table S2. Ten performance metrics for all 84 stacked ensemble models on the validation set

Model	Accuracy	Balanced accuracy	Brier score	F1 score	NPV	PPV	Sensitivity	Specificity	PR-AUC	ROC-AUC
LR + SVM + ENet	0.796	0.796	0.161	0.799	0.794	0.799	0.799	0.794	0.86	0.839
NB + KNN + ENet	0.783	0.784	0.16	0.775	0.754	0.818	0.736	0.832	0.86	0.838
LR + NB + ENet	0.783	0.783	0.16	0.788	0.784	0.783	0.792	0.774	0.861	0.838
SVM + ENet + NNet	0.796	0.796	0.161	0.797	0.79	0.803	0.792	0.8	0.86	0.837
LR + KNN + ENet	0.79	0.79	0.162	0.781	0.76	0.825	0.742	0.839	0.859	0.836
DT + LR + ENet	0.78	0.781	0.163	0.774	0.756	0.808	0.742	0.819	0.858	0.836
NB + SVM + ENet	0.79	0.79	0.159	0.788	0.776	0.804	0.774	0.806	0.859	0.836
DT + NB + ENet	0.78	0.78	0.161	0.785	0.783	0.778	0.792	0.768	0.86	0.836
DT + LR + SVM	0.79	0.789	0.162	0.798	0.803	0.778	0.818	0.761	0.858	0.836
NB + ENet + NNet	0.78	0.781	0.162	0.772	0.753	0.812	0.736	0.826	0.859	0.835
KNN + SVM + ENet	0.783	0.783	0.162	0.785	0.777	0.79	0.78	0.787	0.86	0.835
DT + LR + NB	0.787	0.786	0.161	0.793	0.793	0.78	0.805	0.768	0.856	0.835
DT + ENet + NNet	0.777	0.777	0.163	0.785	0.789	0.766	0.805	0.748	0.857	0.835
LR + NB + KNN	0.783	0.784	0.161	0.77	0.746	0.832	0.717	0.852	0.853	0.834
DT + SVM + ENet	0.79	0.79	0.162	0.795	0.795	0.785	0.805	0.774	0.857	0.834
LR + ENet + NNet	0.777	0.778	0.166	0.76	0.735	0.835	0.698	0.858	0.854	0.833
LR + NB + SVM	0.79	0.79	0.16	0.788	0.776	0.804	0.774	0.806	0.854	0.833
LR + KNN + SVM	0.793	0.794	0.162	0.785	0.765	0.826	0.748	0.839	0.85	0.832
DT + KNN + ENet	0.783	0.784	0.164	0.776	0.757	0.814	0.742	0.826	0.857	0.832
DT + LR + KNN	0.787	0.787	0.163	0.776	0.753	0.829	0.73	0.845	0.849	0.831
KNN + Enet + NNet	0.774	0.775	0.164	0.764	0.744	0.81	0.723	0.826	0.856	0.83
NB + KNN + SVM	0.78	0.781	0.162	0.778	0.765	0.796	0.761	0.8	0.843	0.83
LR + SVM + NNet	0.787	0.787	0.166	0.787	0.778	0.795	0.78	0.794	0.852	0.83
DT + NB + KNN	0.777	0.778	0.163	0.767	0.746	0.816	0.723	0.832	0.845	0.828
DT + NB + NNet	0.783	0.783	0.164	0.788	0.784	0.783	0.792	0.774	0.853	0.828
LR + NB + NNet	0.777	0.778	0.166	0.767	0.746	0.816	0.723	0.832	0.848	0.826
DT + NB + SVM	0.787	0.787	0.162	0.783	0.768	0.807	0.761	0.813	0.839	0.826
DT + LR + NNet	0.768	0.767	0.171	0.771	0.766	0.769	0.774	0.761	0.847	0.826
KNN + SVM + NNet	0.774	0.775	0.165	0.763	0.741	0.814	0.717	0.832	0.84	0.825
DT + SVM + NNet	0.793	0.793	0.163	0.799	0.8	0.787	0.811	0.774	0.836	0.825
NB + KNN + NNet	0.774	0.775	0.165	0.763	0.741	0.814	0.717	0.832	0.836	0.824
NB + SVM + NNet	0.783	0.783	0.164	0.786	0.781	0.786	0.786	0.781	0.835	0.824
LR + KNN + NNet	0.78	0.781	0.17	0.769	0.747	0.821	0.723	0.839	0.846	0.823
DT + KNN + NNet	0.771	0.771	0.168	0.766	0.752	0.792	0.742	0.8	0.842	0.823
NB + RF + ENet	0.783	0.785	0.17	0.764	0.735	0.853	0.692	0.877	0.839	0.818
DT + KNN + SVM	0.758	0.758	0.172	0.761	0.755	0.761	0.761	0.755	0.825	0.816
RF + KNN + ENet	0.78	0.781	0.173	0.761	0.734	0.846	0.692	0.871	0.835	0.815
NB + RF + KNN	0.783	0.785	0.172	0.764	0.735	0.853	0.692	0.877	0.828	0.814
NB + RF + SVM	0.783	0.785	0.173	0.764	0.735	0.853	0.692	0.877	0.829	0.813
RF + SVM + ENet	0.777	0.778	0.173	0.755	0.727	0.85	0.679	0.877	0.834	0.813

LR + NB + RF	0.783	0.785	0.173	0.759	0.728	0.87	0.673	0.897	0.827	0.811
LR + RF + ENet	0.774	0.775	0.175	0.746	0.716	0.867	0.654	0.897	0.835	0.811
DT + NB + RF	0.78	0.782	0.172	0.754	0.724	0.869	0.667	0.897	0.829	0.81
DT + RF + ENet	0.774	0.775	0.174	0.746	0.716	0.867	0.654	0.897	0.833	0.81
LR + RF + SVM	0.78	0.781	0.175	0.761	0.734	0.846	0.692	0.871	0.814	0.809
LR + RF + KNN	0.771	0.772	0.175	0.741	0.713	0.866	0.648	0.897	0.816	0.808
DT + LR + RF	0.774	0.775	0.175	0.746	0.716	0.867	0.654	0.897	0.819	0.806
RF + KNN + SVM	0.768	0.769	0.178	0.74	0.714	0.852	0.654	0.884	0.813	0.804
DT + RF + SVM	0.771	0.772	0.178	0.741	0.713	0.866	0.648	0.897	0.809	0.802
DT + RF + KNN	0.768	0.769	0.179	0.747	0.723	0.831	0.679	0.858	0.813	0.801
RF + ENet + NNet	0.752	0.753	0.182	0.713	0.692	0.858	0.61	0.897	0.824	0.799
RF + ENet + XGB	0.748	0.749	0.189	0.729	0.709	0.803	0.667	0.832	0.809	0.796
RF + SVM + NNet	0.768	0.769	0.183	0.736	0.709	0.864	0.642	0.897	0.792	0.795
NB + RF + NNet	0.768	0.769	0.182	0.746	0.72	0.836	0.673	0.865	0.818	0.795
KNN + ENet + XGB	0.745	0.746	0.189	0.72	0.701	0.811	0.648	0.845	0.81	0.795
RF + KNN + XGB	0.748	0.749	0.189	0.736	0.718	0.786	0.692	0.806	0.795	0.795
DT + RF + NNet	0.764	0.766	0.184	0.739	0.714	0.84	0.66	0.871	0.8	0.794
KNN + SVM + XGB	0.745	0.747	0.19	0.718	0.698	0.816	0.642	0.852	0.794	0.794
SVM + ENet + XGB	0.748	0.75	0.191	0.725	0.704	0.812	0.654	0.845	0.806	0.793
RF + SVM + XGB	0.748	0.75	0.19	0.727	0.707	0.808	0.66	0.839	0.785	0.793
NB + ENet + XGB	0.748	0.75	0.192	0.725	0.704	0.812	0.654	0.845	0.812	0.792
NB + KNN + XGB	0.745	0.746	0.191	0.735	0.719	0.776	0.698	0.794	0.799	0.791
NB + RF + XGB	0.745	0.747	0.191	0.716	0.696	0.821	0.635	0.858	0.789	0.789
RF + KNN + NNet	0.755	0.756	0.188	0.724	0.701	0.842	0.635	0.877	0.8	0.788
NB + SVM + XGB	0.742	0.743	0.192	0.714	0.695	0.815	0.635	0.852	0.784	0.788
LR + RF + NNet	0.755	0.756	0.186	0.739	0.719	0.801	0.686	0.826	0.812	0.788
LR + ENet + XGB	0.736	0.737	0.196	0.713	0.696	0.792	0.648	0.826	0.81	0.788
LR + NB + XGB	0.748	0.75	0.193	0.723	0.702	0.817	0.648	0.852	0.801	0.786
LR + KNN + XGB	0.745	0.746	0.192	0.732	0.714	0.784	0.686	0.806	0.789	0.785
LR + RF + XGB	0.742	0.743	0.193	0.714	0.695	0.815	0.635	0.852	0.776	0.783
DT + KNN + XGB	0.739	0.74	0.193	0.715	0.697	0.798	0.648	0.832	0.799	0.783
DT + ENet + XGB	0.736	0.736	0.198	0.722	0.707	0.771	0.679	0.794	0.808	0.783
LR + SVM + XGB	0.745	0.746	0.194	0.737	0.722	0.772	0.704	0.787	0.773	0.783
ENet + NNet + XGB	0.726	0.726	0.201	0.724	0.714	0.739	0.711	0.742	0.804	0.781
DT + SVM + XGB	0.739	0.739	0.196	0.732	0.719	0.762	0.704	0.774	0.785	0.78
DT + LR + XGB	0.739	0.74	0.198	0.725	0.709	0.777	0.679	0.8	0.799	0.779
DT + NB + XGB	0.739	0.74	0.196	0.711	0.693	0.808	0.635	0.845	0.802	0.778
NB + NNet + XGB	0.739	0.74	0.196	0.713	0.695	0.803	0.642	0.839	0.8	0.778
LR + NNet + XGB	0.726	0.727	0.204	0.697	0.683	0.792	0.623	0.832	0.796	0.778
DT + RF + XGB	0.742	0.743	0.196	0.725	0.708	0.787	0.673	0.813	0.781	0.777
KNN + NNet + XGB	0.729	0.731	0.199	0.686	0.673	0.83	0.585	0.877	0.775	0.774
DT + NNet + XGB	0.736	0.737	0.201	0.717	0.7	0.784	0.66	0.813	0.78	0.77
SVM + NNet + XGB	0.732	0.733	0.201	0.729	0.718	0.748	0.711	0.755	0.743	0.769
RF + NNet + XGB	0.723	0.723	0.2	0.718	0.707	0.74	0.698	0.748	0.749	0.769

NPV, negative predictive value; PPV, positive predictive value; PR-AUC, the area under the precision recall curve; ROC-AUC, the area under the receiver operating characteristic curve; DT, decision tree; LR, logistic regression; NB, naive Bayes; RF, random forest; KNN, k-nearest neighbor; SVM, support vector machine; Enet, elastic net regression; NNet, neural network; XGB, extreme gradient boosting.