Supplementary Table 1. Global and per-target correlation coefficients for the MCC scores versus the BDT scores using different values for d_0 (1, 2, 3, 5, 7, 9). "FN_1" is used to indicate results where only the FN_1 prediction scores from each group have been used; "all FN" is used to indicate results where all prediction scores (FN_1 to FN_5) have been used from each group

	Pearson MCC vs BDT 1	Pearson MCC vs BDT 2	Pearson MCC vs BDT 3
Global all FN	0.9658	0.9634	0.9547
Global FN_1	0.9653	0.9642	0.9579

	Pearson MCC vs BDT 5	Pearson MCC vs BDT 7	Pearson MCC vs BDT 9
Global all FN	0.9224	0.8817	0.8387
Global FN_1	0.9320	0.8976	0.8604

	Spearman MCC vs BDT 1	Spearman MCC vs BDT 2	Spearman MCC vs BDT 3
Global all FN	0.9276	0.9142	0.8925
Global FN_1	0.9596	0.9523	0.9388

	Spearman MCC vs BDT 5	Spearman MCC vs BDT 7	Spearman MCC vs BDT 9
Global all FN	0.8482	0.8103	0.7776
Global FN_1	0.9081	0.8772	0.8490

	Kendall MCC vs BDT 1	Kendall MCC vs BDT 2	Kendall MCC vs BDT 3
Global all FN	0.7638	0.7455	0.7175
Global FN_1	0.8202	0.8059	0.7832

	Kendall MCC vs BDT 5	Kendall MCC vs BDT 7	Kendall MCC vs BDT 9
Global all FN	0.6631	0.6186	0.5828
Global FN_1	0.7364	0.6942	0.6611

Per-target all FN

Target	Pearson MCC vs BDT 1	Pearson MCC vs BDT 2	Pearson MCC vs BDT 3
T0391	0.9816	0.9789	0.9725
T0394	0.9754	0.9746	0.9679
T0396	0.9498	0.9312	0.9033
T0406	0.9703	0.9731	0.9714
T0407	0.9727	0.9715	0.9608
T0410	0.9792	0.9770	0.9724
T0422	0.9878	0.9873	0.9851
T0425	0.9604	0.9623	0.9591
T0426	0.9482	0.9546	0.9603
T0430	0.9870	0.9846	0.9794
T0431	0.9841	0.9739	0.9521
T0440	0.9664	0.9664	0.9593
T0444	0.9670	0.9719	0.9723
T0450	0.9886	0.9863	0.9815
T0453	0.9818	0.9782	0.9674
T0457	0.9524	0.9558	0.9508
T0461	0.9380	0.9448	0.9443
T0470	0.9606	0.9648	0.9662
T0476	0.9652	0.9386	0.8871
T0477	0.9762	0.9776	0.9761
T0478	0.9115	0.9009	0.8796
T0480	0.9791	0.9691	0.9437
T0483	0.9824	0.9785	0.9710

Target			
T0485	0.9786	0.9704	0.9561
T0487	0.9004	0.6470	0.4225
T0490	0.9710	0.9621	0.9473
T0508	0.9798	0.9739	0.9628
mean	0.9665	0.9539	0.9360

Target	Pearson MCC vs BDT 5	Pearson MCC vs BDT 7	Pearson MCC vs BDT 9
T0391	0.9503	0.9190	0.8799
T0394	0.9404	0.9038	0.8628
T0396	0.8408	0.7872	0.7457
T0406	0.9526	0.9219	0.8858
T0407	0.9115	0.8446	0.7761
T0410	0.9589	0.9419	0.9216
T0422	0.9746	0.9579	0.9356
T0425	0.9348	0.8996	0.8640
T0426	0.9619	0.9503	0.9292
T0430	0.9623	0.9381	0.9079
T0431	0.8892	0.8232	0.7621
T0440	0.9166	0.8480	0.7712
T0444	0.9577	0.9314	0.8999
T0450	0.9659	0.9452	0.9222
T0453	0.9239	0.8620	0.7922
T0457	0.9242	0.8935	0.8653
T0461	0.9229	0.8941	0.8675
T0470	0.9524	0.9215	0.8827
T0476	0.7963	0.7383	0.6959
T0477	0.9663	0.9514	0.9333
T0478	0.8328	0.7858	0.7385
T0480	0.8680	0.7990	0.7487
T0483	0.9461	0.9119	0.8714
T0485	0.9167	0.8749	0.8364
T0487	0.2312	0.1570	0.1180
T0490	0.9059	0.8577	0.8100
T0508	0.9288	0.8874	0.8446
mean	0.8975	0.8573	0.8174

Target	Spearman MCC vs BDT 1	Spearman MCC vs BDT 2	Spearman MCC vs BDT 3
T0391	0.8955	0.8940	0.8899
T0394	0.9079	0.9050	0.8992
T0396	0.9381	0.9205	0.8723
T0406	0.9632	0.9482	0.9326
T0407	0.9231	0.9009	0.8343
T0410	0.9625	0.9620	0.9458
T0422	0.9553	0.9553	0.9536
T0425	0.8989	0.8838	0.8643
T0426	0.8749	0.8738	0.8678
T0430	0.9332	0.9280	0.9010
T0431	0.9577	0.9392	0.9187
T0440	0.9354	0.9356	0.9277
T0444	0.6968	0.6963	0.6853
T0450	0.9554	0.9575	0.9412
T0453	0.3505	0.3463	0.3412
T0457	0.8983	0.8955	0.8911
T0461	0.9406	0.9332	0.9176
T0470	0.9327	0.9384	0.9329
T0476	0.7176	0.7142	0.6778

Target			
T0477	0.9540	0.9478	0.9421
T0478	0.5721	0.5677	0.5579
T0480	0.8906	0.8741	0.8646
T0483	0.9263	0.9184	0.8909
T0485	0.9286	0.9159	0.9011
T0487	0.6099	0.4982	0.4300
T0490	0.8916	0.8666	0.8268
T0508	0.9699	0.9620	0.9497
mean	0.8660	0.8548	0.8355

Target	Spearman MCC vs BDT 5	Spearman MCC vs BDT 7	Spearman MCC vs BDT 9
T0391	0.8770	0.8589	0.8172
T0394	0.8750	0.8370	0.8038
T0396	0.8278	0.7873	0.7585
T0406	0.8960	0.8682	0.8314
T0407	0.7599	0.6977	0.6562
T0410	0.9410	0.9051	0.8822
T0422	0.9486	0.9388	0.9267
T0425	0.8249	0.8170	0.8120
T0426	0.8586	0.8438	0.8256
T0430	0.8409	0.7866	0.7647
T0431	0.8704	0.8218	0.7858
T0440	0.8632	0.8076	0.7352
T0444	0.6647	0.6493	0.6352
T0450	0.9240	0.9069	0.8914
T0453	0.3116	0.2944	0.2727
T0457	0.8818	0.8775	0.8611
T0461	0.8765	0.8652	0.8556
T0470	0.9151	0.8948	0.8563
T0476	0.6280	0.6029	0.5679
T0477	0.9241	0.9183	0.8874
T0478	0.5294	0.5066	0.4901
T0480	0.8172	0.7791	0.7665
T0483	0.8428	0.7904	0.7525
T0485	0.8552	0.8207	0.8115
T0487	0.3256	0.3013	0.2502
T0490	0.7730	0.7364	0.7080
T0508	0.9252	0.8968	0.8629
mean	0.7992	0.7708	0.7433

Target	Kendall MCC vs BDT 1	Kendall MCC vs BDT 2	Kendall MCC vs BDT 3
T0391	0.7479	0.7412	0.7277
T0394	0.7312	0.7261	0.7108
T0396	0.7954	0.7637	0.7098
T0406	0.8591	0.8228	0.8015
T0407	0.7881	0.7579	0.6834
T0410	0.8675	0.8645	0.8174
T0422	0.8284	0.8284	0.8147
T0425	0.7645	0.7427	0.7236
T0426	0.7189	0.7155	0.6950
T0430	0.7954	0.7844	0.7530
T0431	0.8236	0.7772	0.7327
T0440	0.8154	0.8103	0.7897
T0444	0.5288	0.5273	0.5068
T0450	0.8198	0.8259	0.8077
T0453	0.2196	0.2161	0.2108

Target			
T0457	0.7623	0.7516	0.7409
T0461	0.8140	0.7980	0.7688
T0470	0.7914	0.8096	0.7966
T0476	0.5552	0.5455	0.5037
T0477	0.8293	0.8114	0.8025
T0478	0.3384	0.3244	0.3337
T0480	0.7413	0.7069	0.6832
T0483	0.8044	0.7840	0.7461
T0485	0.7738	0.7542	0.7315
T0487	0.4640	0.3555	0.3012
T0490	0.7308	0.7005	0.6613
T0508	0.8573	0.8398	0.8160
mean	0.7247	0.7069	0.6804

Target	Kendall MCC vs BDT 7	Kendall MCC vs BDT 5	Kendall MCC vs BDT 9
T0391	0.6738	0.7030	0.6222
T0394	0.6237	0.6698	0.5879
T0396	0.6149	0.6595	0.5851
T0406	0.7097	0.7567	0.6734
T0407	0.5483	0.6182	0.5064
T0410	0.7408	0.8115	0.7084
T0422	0.7925	0.8096	0.7599
T0425	0.6799	0.6853	0.6690
T0426	0.6590	0.6795	0.6418
T0430	0.6161	0.6743	0.5972
T0431	0.5892	0.6579	0.5447
T0440	0.6328	0.7048	0.5582
T0444	0.4745	0.4877	0.4584
T0450	0.7653	0.7865	0.7441
T0453	0.1638	0.1795	0.1377
T0457	0.7132	0.7260	0.6962
T0461	0.7017	0.7192	0.6944
T0470	0.7394	0.7706	0.6927
T0476	0.4200	0.4522	0.3910
T0477	0.7775	0.7829	0.7383
T0478	0.2964	0.3057	0.2964
T0480	0.5722	0.6144	0.5589
T0483	0.6135	0.6776	0.5712
T0485	0.6362	0.6755	0.6241
T0487	0.2144	0.2280	0.1791
T0490	0.5634	0.6115	0.5260
T0508	0.7240	0.7685	0.6765
mean	0.6021	0.6376	0.5718

Per-target FN_1

Target	Pearson MCC vs BDT 1	PearsonMCC vs BDT 2	Pearson MCC vs BDT 3
T0391	0.9785	0.9726	0.9614
T0394	0.9776	0.9727	0.9605
T0396	0.9802	0.9718	0.9581
T0406	0.9727	0.9807	0.9858
T0407	0.9888	0.9876	0.9805
T0410	0.9747	0.9739	0.9715
T0422	0.9890	0.9906	0.9918
T0425	0.9598	0.9654	0.9707
T0426	0.9607	0.9653	0.9709
T0430	0.9832	0.9780	0.9693

Target			
T0431	0.9580	0.9333	0.8898
T0440	0.9733	0.9681	0.9535
T0444	0.9568	0.9665	0.9736
T0450	0.9907	0.9881	0.9830
T0453	0.9754	0.9647	0.9398
T0457	0.9517	0.9564	0.9528
T0461	0.9456	0.9546	0.9624
T0470	0.9598	0.9677	0.9745
T0476	0.9672	0.9130	0.8288
T0477	0.9670	0.9713	0.9734
T0478	0.9308	0.9435	0.9519
T0480	0.9925	0.9885	0.9766
T0483	0.9900	0.9841	0.9722
T0485	0.9911	0.9864	0.9774
T0487	0.9561	0.7278	0.4171
T0490	0.9756	0.9669	0.9530
T0508	0.9791	0.9741	0.9648
mean	0.9713	0.9598	0.9395

Target	Pearson MCC vs BDT 5	Pearson MCC vs BDT 7	Pearson MCC vs BDT 9
T0391	0.9240	0.8702	0.8022
T0394	0.9254	0.8890	0.8539
T0396	0.9247	0.8946	0.8709
T0406	0.9823	0.9683	0.9516
T0407	0.9465	0.8981	0.8482
T0410	0.9638	0.9549	0.9449
T0422	0.9912	0.9867	0.9791
T0425	0.9722	0.9608	0.9425
T0426	0.9792	0.9814	0.9787
T0430	0.9436	0.9083	0.8639
T0431	0.7760	0.6634	0.5639
T0440	0.8893	0.7895	0.6745
T0444	0.9715	0.9558	0.9357
T0450	0.9665	0.9445	0.9197
T0453	0.8599	0.7719	0.6928
T0457	0.9332	0.9141	0.8982
T0461	0.9660	0.9585	0.9476
T0470	0.9751	0.9603	0.9377
T0476	0.7005	0.6309	0.5881
T0477	0.9700	0.9616	0.9519
T0478	0.9495	0.9234	0.8792
T0480	0.9338	0.8857	0.8436
T0483	0.9332	0.8827	0.8267
T0485	0.9499	0.9185	0.8888
T0487	0.1031	-0.0167	-0.0765
T0490	0.9138	0.8653	0.8133
T0508	0.9368	0.9020	0.8638
mean	0.8993	0.8601	0.8217

Target	Spearman MCC vs BDT 1	Spearman MCC vs BDT 2	Spearman MCC vs BDT 3
T0391	0.9429	0.9429	0.9306
T0394	0.9816	0.9787	0.9669
T0396	0.9825	0.9772	0.9737
T0406	0.9955	0.9955	0.9955
T0407	0.9519	0.9409	0.8996
T0410	0.9301	0.9301	0.9014

Target			
T0422	0.9848	0.9848	0.9812
T0425	0.9350	0.9350	0.9350
T0426	0.9454	0.9543	0.9543
T0430	0.7758	0.7670	0.7275
T0431	0.9604	0.9297	0.8813
T0440	0.9428	0.9463	0.9284
T0444	0.8179	0.8143	0.8143
T0450	0.9464	0.9500	0.9071
T0453	0.1432	0.1314	0.1314
T0457	0.9205	0.9133	0.8990
T0461	0.9405	0.9552	0.9503
T0470	0.9890	0.9945	0.9945
T0476	0.8996	0.8859	0.8722
T0477	0.9848	0.9777	0.9741
T0478	0.5422	0.5422	0.5422
T0480	0.9267	0.9267	0.9222
T0483	0.9679	0.9643	0.9429
T0485	0.9295	0.9295	0.9295
T0487	0.8807	0.6912	0.5895
T0490	0.9175	0.8910	0.8527
T0508	0.9639	0.9580	0.9433
mean	0.8925	0.8818	0.8645

Target	Spearman MCC vs BDT 5	Spearman MCC vs BDT 7	Spearman MCC vs BDT 9
T0391	0.9134	0.8766	0.8422
T0394	0.9169	0.8477	0.8153
T0396	0.9456	0.9035	0.8895
T0406	0.9919	0.9740	0.9615
T0407	0.8748	0.8061	0.8006
T0410	0.9014	0.8943	0.8943
T0422	0.9812	0.9812	0.9812
T0425	0.9561	0.9701	0.9596
T0426	0.9526	0.9615	0.9615
T0430	0.6879	0.6879	0.6659
T0431	0.7538	0.6352	0.5253
T0440	0.8640	0.7710	0.6100
T0444	0.8071	0.8071	0.7857
T0450	0.9143	0.9107	0.9107
T0453	0.0797	0.0413	-0.0339
T0457	0.8811	0.8740	0.8740
T0461	0.9478	0.9454	0.9454
T0470	0.9890	0.9725	0.9614
T0476	0.7854	0.6758	0.6210
T0477	0.9651	0.9634	0.9598
T0478	0.5181	0.5904	0.5904
T0480	0.9222	0.9222	0.9222
T0483	0.9250	0.9179	0.8714
T0485	0.8987	0.8943	0.8943
T0487	0.3298	0.2561	0.2070
T0490	0.8527	0.8380	0.8262
T0508	0.9020	0.8489	0.8430
mean	0.8318	0.8062	0.7809

Target	Kendall MCC vs BDT 1	Kendall MCC vs BDT 2	Kendall MCC vs BDT 3
T0391	0.8327	0.8327	0.8179
T0394	0.9121	0.8954	0.8619

Target			
T0396	0.9064	0.8947	0.8830
T0406	0.9759	0.9759	0.9759
T0407	0.8645	0.8387	0.7871
T0410	0.8156	0.8156	0.7379
T0422	0.9372	0.9372	0.9179
T0425	0.8372	0.8372	0.8372
T0426	0.8406	0.8599	0.8599
T0430	0.6264	0.6044	0.5604
T0431	0.8681	0.7802	0.6923
T0440	0.8269	0.8462	0.7885
T0444	0.6571	0.6381	0.6381
T0450	0.8095	0.8286	0.7714
T0453	0.0681	0.0511	0.0511
T0457	0.8038	0.7847	0.7464
T0461	0.8625	0.8625	0.8476
T0470	0.9481	0.9740	0.9740
T0476	0.7964	0.7594	0.7223
T0477	0.9378	0.9187	0.8995
T0478	0.3333	0.3333	0.3333
T0480	0.8276	0.8276	0.8047
T0483	0.9048	0.8857	0.8476
T0485	0.8222	0.8222	0.8222
T0487	0.7385	0.5231	0.4000
T0490	0.7647	0.7311	0.6975
T0508	0.8776	0.8608	0.8270
mean	0.7924	0.7748	0.7445

Target	Kendall MCC vs BDT 5	Kendall MCC vs BDT 7	Kendall MCC vs BDT 9
T0391	0.7881	0.7286	0.6840
T0394	0.7615	0.6611	0.6276
T0396	0.8363	0.7661	0.7427
T0406	0.9565	0.8986	0.8599
T0407	0.7871	0.7097	0.6839
T0410	0.7379	0.7379	0.7379
T0422	0.9179	0.9179	0.9179
T0425	0.8993	0.8993	0.8682
T0426	0.8599	0.8792	0.8792
T0430	0.5165	0.5165	0.4725
T0431	0.5824	0.4505	0.3407
T0440	0.7115	0.6346	0.5000
T0444	0.6190	0.6190	0.6000
T0450	0.7905	0.7905	0.7905
T0453	0.0170	-0.0340	-0.0851
T0457	0.7273	0.7081	0.7081
T0461	0.8327	0.8179	0.8179
T0470	0.9481	0.8961	0.8701
T0476	0.6112	0.5001	0.4630
T0477	0.8995	0.8804	0.8613
T0478	0.2593	0.4074	0.4074
T0480	0.8047	0.8047	0.8047
T0483	0.8095	0.7905	0.7333
T0485	0.7778	0.7556	0.7556
T0487	0.2154	0.1539	0.1231
T0490	0.6975	0.6639	0.6471
T0508	0.7595	0.6582	0.6414
mean	0.7083	0.6745	0.6464