



Figure S1. Univariate feature score plots from the selected EBM model, showing the features with minimal impact. The blue line shows the EBM score across value bins, where each bin represents a range of feature values. Orange bars indicate the number of samples in each bin. Gray shaded regions mark areas with limited or no data, where the model extrapolates. Larger gray regions indicate lower reliability of the score in those ranges.

Table S1. Results of all trials (7 feature combinations) using MIC threshold = 10 μ M.

trials	features	cross validation	training							test						
		F1	balanced accuracy	F1	precision	recall	AUC-ROC	AUC-PR	MCC	balanced accuracy	F1	precision	recall	AUC-ROC	AUC-PR	MCC
CTD_global	9	0.7744	0.8714	0.8656	0.8621	0.869	0.9461	0.9435	0.7425	0.7521	0.7417	0.7358	0.7476	0.8365	0.8237	0.5038
composition_global	11	0.7592	0.8091	0.8074	0.7697	0.849	0.8968	0.8873	0.6183	0.7312	0.7295	0.6957	0.7668	0.8145	0.7921	0.4624
composition_CTD	13	0.7733	0.8521	0.8477	0.8274	0.869	0.9291	0.9168	0.7035	0.7309	0.7204	0.7125	0.7284	0.8129	0.7864	0.4614
global	4	0.7316	0.8026	0.7956	0.7833	0.8083	0.8956	0.891	0.6045	0.753	0.7465	0.7273	0.7668	0.8242	0.8064	0.5053
CTD	13	0.7771	0.8715	0.8673	0.8481	0.8874	0.9452	0.9386	0.7421	0.7602	0.7524	0.7385	0.7668	0.8353	0.8166	0.5198
composition	10	0.7568	0.8008	0.8015	0.7533	0.8562	0.8764	0.8547	0.6029	0.7246	0.7273	0.6816	0.7796	0.7837	0.7711	0.4503
composition_CTD_global	12	0.7894	0.8661	0.8602	0.8555	0.865	0.9381	0.9331	0.7319	0.7616	0.7535	0.7407	0.7668	0.8322	0.8024	0.5227

Table S2. Results of all trials (7 feature combinations) using MIC threshold = 15 μ M.

trials	features	cross validation	training							test						
		F1	balanced accuracy	F1	precision	recall	AUC-ROC	AUC-PR	MCC	balanced accuracy	F1	precision	recall	AUC-ROC	AUC-PR	MCC
CTD_global	13	0.8332	0.8469	0.8762	0.8537	0.9	0.9336	0.9492	0.7017	0.7574	0.8015	0.7816	0.8225	0.8243	0.8533	0.5203
composition_global	7	0.8097	0.7992	0.8444	0.8031	0.8902	0.8908	0.9114	0.6148	0.732	0.7916	0.75	0.8381	0.7864	0.8062	0.4782
composition_CTD	7	0.809	0.7855	0.8392	0.7845	0.902	0.8835	0.9062	0.5953	0.7006	0.7713	0.7221	0.8277	0.7738	0.8153	0.4178
global	3	0.7924	0.7615	0.8179	0.7691	0.8732	0.846	0.8693	0.5423	0.7088	0.7766	0.7294	0.8303	0.7883	0.8027	0.4337
CTD	11	0.8199	0.8324	0.8678	0.835	0.9033	0.9161	0.9317	0.6773	0.7391	0.7831	0.7702	0.7963	0.8109	0.8407	0.4813
composition	8	0.8106	0.7801	0.8336	0.7822	0.8922	0.872	0.8927	0.5821	0.7053	0.7778	0.7236	0.8407	0.7793	0.8116	0.4305
composition_CTD_global	9	0.8213	0.8332	0.8672	0.8379	0.8987	0.9214	0.9386	0.6771	0.7565	0.8025	0.7789	0.8277	0.8355	0.8563	0.5199

Table S3. Performance metrics of all hyperparameter trial models across the folds of 5-fold cross-validation.

dropout rate	learning rate	label smoothing factor	weight decay	balanced accuracy	F1	precision	recall	AUC-ROC	AUC-PR	MCC	loss	fold
0.1	5.00E-06	0	0	0.8025	0.8415	0.8152	0.8696	0.8567	0.8511	0.6139	0.4673	fold_1
0.1	5.00E-06	0	0.01	0.7928	0.8295	0.8134	0.8464	0.8572	0.8681	0.5905	0.4646	fold_1
0.1	5.00E-06	0.1	0	0.7932	0.8382	0.8016	0.8783	0.8473	0.8575	0.6001	0.5128	fold_1
0.1	5.00E-06	0.1	0.01	0.7933	0.8352	0.8059	0.8667	0.8609	0.8776	0.5966	0.5153	fold_1
0.1	1.00E-05	0	0	0.8182	0.8421	0.8496	0.8348	0.8815	0.8966	0.6346	0.4321	fold_1
0.1	1.00E-05	0	0.01	0.8098	0.8467	0.8224	0.8725	0.8626	0.8703	0.6277	0.4568	fold_1
0.1	1.00E-05	0.1	0	0.7865	0.8234	0.8095	0.8377	0.8486	0.8544	0.577	0.5176	fold_1
0.1	1.00E-05	0.1	0.01	0.7924	0.8237	0.8213	0.8261	0.865	0.8827	0.5854	0.5131	fold_1
0.3	5.00E-06	0	0	0.7841	0.8195	0.8102	0.829	0.8349	0.8467	0.5708	0.485	fold_1
0.3	5.00E-06	0	0.01	0.7806	0.8261	0.7941	0.8609	0.8331	0.8202	0.5723	0.4962	fold_1
0.3	5.00E-06	0.1	0	0.8035	0.8376	0.8235	0.8522	0.859	0.8694	0.6112	0.5091	fold_1
0.3	5.00E-06	0.1	0.01	0.7898	0.8354	0.7989	0.8754	0.8552	0.8671	0.5932	0.5142	fold_1
0.3	1.00E-05	0	0	0.7928	0.8357	0.8043	0.8696	0.867	0.881	0.5965	0.4623	fold_1
0.3	1.00E-05	0	0.01	0.8151	0.8507	0.8274	0.8754	0.8754	0.8973	0.638	0.451	fold_1
0.3	1.00E-05	0.1	0	0.8006	0.8343	0.8225	0.8464	0.8532	0.8581	0.6046	0.5189	fold_1
0.3	1.00E-05	0.1	0.01	0.8121	0.8532	0.817	0.8928	0.8547	0.856	0.6382	0.5066	fold_1
0.5	5.00E-06	0	0	0.8059	0.8443	0.8179	0.8725	0.858	0.8615	0.6208	0.4822	fold_1
0.5	5.00E-06	0	0.01	0.7968	0.8256	0.828	0.8232	0.8529	0.8793	0.593	0.4858	fold_1
0.5	5.00E-06	0.1	0	0.7772	0.8264	0.7874	0.8696	0.8274	0.834	0.5689	0.5397	fold_1
0.5	5.00E-06	0.1	0.01	0.8045	0.8397	0.8222	0.858	0.8514	0.8568	0.6143	0.5224	fold_1
0.5	1.00E-05	0	0	0.7796	0.8271	0.791	0.8667	0.8471	0.858	0.5723	0.4888	fold_1
0.5	1.00E-05	0	0.01	0.8072	0.8544	0.8051	0.9101	0.8594	0.8673	0.6363	0.4546	fold_1
0.5	1.00E-05	0.1	0	0.7942	0.8373	0.8048	0.8725	0.8477	0.8471	0.6	0.5178	fold_1
0.5	1.00E-05	0.1	0.01	0.7967	0.835	0.8132	0.858	0.8519	0.8615	0.6003	0.5213	fold_1
0.1	5.00E-06	0	0	0.7873	0.8255	0.8061	0.8459	0.8483	0.8556	0.5804	0.4859	fold_2
0.1	5.00E-06	0	0.01	0.7689	0.8097	0.7917	0.8285	0.8331	0.8586	0.5428	0.5074	fold_2
0.1	5.00E-06	0.1	0	0.7825	0.821	0.8028	0.8401	0.8488	0.8684	0.5702	0.5333	fold_2

0.1	5.00E-06	0.1	0.01	0.7786	0.8187	0.7983	0.8401	0.8487	0.8677	0.5631	0.5335	fold_2
0.1	1.00E-05	0	0	0.8043	0.8397	0.8199	0.8605	0.8546	0.86	0.6146	0.4673	fold_2
0.1	1.00E-05	0	0.01	0.7994	0.829	0.8266	0.8314	0.8594	0.8798	0.5994	0.4791	fold_2
0.1	1.00E-05	0.1	0	0.797	0.8345	0.8127	0.8576	0.8413	0.8491	0.6008	0.5231	fold_2
0.1	1.00E-05	0.1	0.01	0.7999	0.8348	0.8184	0.8517	0.8386	0.8444	0.6046	0.5267	fold_2
0.3	5.00E-06	0	0	0.782	0.8117	0.8152	0.8081	0.8446	0.8651	0.5632	0.5029	fold_2
0.3	5.00E-06	0	0.01	0.7796	0.8144	0.8063	0.8227	0.8373	0.8551	0.5612	0.4989	fold_2
0.3	5.00E-06	0.1	0	0.796	0.8384	0.8048	0.875	0.8462	0.85	0.604	0.5273	fold_2
0.3	5.00E-06	0.1	0.01	0.7781	0.8255	0.7884	0.8663	0.8338	0.8509	0.5694	0.5388	fold_2
0.3	1.00E-05	0	0	0.7999	0.8348	0.8184	0.8517	0.8562	0.875	0.6046	0.474	fold_2
0.3	1.00E-05	0	0.01	0.7965	0.8223	0.8309	0.814	0.8534	0.8681	0.5912	0.482	fold_2
0.3	1.00E-05	0.1	0	0.8033	0.8345	0.8262	0.843	0.8415	0.854	0.6088	0.5264	fold_2
0.3	1.00E-05	0.1	0.01	0.7951	0.8302	0.8151	0.8459	0.8517	0.8673	0.5944	0.522	fold_2
0.5	5.00E-06	0	0	0.7587	0.8204	0.7612	0.8895	0.8287	0.8416	0.5437	0.5172	fold_2
0.5	5.00E-06	0	0.01	0.7641	0.8242	0.7656	0.8924	0.8291	0.8412	0.5542	0.5169	fold_2
0.5	5.00E-06	0.1	0	0.7781	0.8224	0.7925	0.8547	0.8402	0.8455	0.566	0.5376	fold_2
0.5	5.00E-06	0.1	0.01	0.7752	0.8058	0.8094	0.8023	0.8508	0.8733	0.5496	0.5434	fold_2
0.5	1.00E-05	0	0	0.7975	0.8371	0.8098	0.8663	0.8517	0.8683	0.604	0.4843	fold_2
0.5	1.00E-05	0	0.01	0.7926	0.8295	0.8111	0.8488	0.8496	0.8413	0.5907	0.4975	fold_2
0.5	1.00E-05	0.1	0	0.7984	0.83	0.8229	0.8372	0.85	0.8698	0.5988	0.5256	fold_2
0.5	1.00E-05	0.1	0.01	0.7883	0.8113	0.8298	0.7936	0.8414	0.8661	0.5731	0.5362	fold_2
0.1	5.00E-06	0	0	0.7868	0.8229	0.809	0.8372	0.8569	0.8844	0.5775	0.4824	fold_3
0.1	5.00E-06	0	0.01	0.7844	0.819	0.8097	0.8285	0.8569	0.8884	0.5712	0.4753	fold_3
0.1	5.00E-06	0.1	0	0.8091	0.8412	0.8282	0.8547	0.8552	0.8753	0.622	0.511	fold_3
0.1	5.00E-06	0.1	0.01	0.811	0.8424	0.8305	0.8547	0.8565	0.8777	0.6255	0.5067	fold_3
0.1	1.00E-05	0	0	0.7883	0.8397	0.7883	0.8983	0.8556	0.8522	0.5987	0.4583	fold_3
0.1	1.00E-05	0	0.01	0.8052	0.8448	0.814	0.8779	0.8699	0.8681	0.6212	0.4604	fold_3
0.1	1.00E-05	0.1	0	0.8062	0.8409	0.8222	0.8605	0.8832	0.9086	0.6181	0.4995	fold_3
0.1	1.00E-05	0.1	0.01	0.813	0.8436	0.8329	0.8547	0.8666	0.8808	0.629	0.5004	fold_3
0.3	5.00E-06	0	0	0.7883	0.818	0.8192	0.8169	0.859	0.8943	0.5763	0.4846	fold_3

0.3	5.00E-06	0	0.01	0.7994	0.8321	0.8215	0.843	0.8515	0.8676	0.6017	0.4814	fold_3
0.3	5.00E-06	0.1	0	0.8159	0.8499	0.8287	0.8721	0.8629	0.8758	0.6386	0.4993	fold_3
0.3	5.00E-06	0.1	0.01	0.8052	0.8388	0.8235	0.8547	0.8698	0.8931	0.6149	0.5052	fold_3
0.3	1.00E-05	0	0	0.7965	0.835	0.811	0.8605	0.8692	0.8849	0.6007	0.4608	fold_3
0.3	1.00E-05	0	0.01	0.7946	0.8368	0.8043	0.8721	0.8642	0.8794	0.6005	0.4639	fold_3
0.3	1.00E-05	0.1	0	0.8038	0.8341	0.8281	0.8401	0.8574	0.8764	0.6091	0.5145	fold_3
0.3	1.00E-05	0.1	0.01	0.7902	0.8257	0.8118	0.8401	0.8652	0.8758	0.5843	0.505	fold_3
0.5	5.00E-06	0	0	0.7859	0.827	0.8011	0.8547	0.8454	0.8395	0.58	0.5052	fold_3
0.5	5.00E-06	0	0.01	0.781	0.8257	0.7936	0.8605	0.8439	0.8461	0.5729	0.5034	fold_3
0.5	5.00E-06	0.1	0	0.7922	0.8331	0.8049	0.8634	0.8518	0.8745	0.5937	0.5198	fold_3
0.5	5.00E-06	0.1	0.01	0.7936	0.8317	0.8099	0.8547	0.8602	0.8833	0.5939	0.5206	fold_3
0.5	1.00E-05	0	0	0.7955	0.8329	0.8122	0.8547	0.8583	0.8672	0.5974	0.4746	fold_3
0.5	1.00E-05	0	0.01	0.797	0.8345	0.8127	0.8576	0.8605	0.8821	0.6008	0.4731	fold_3
0.5	1.00E-05	0.1	0	0.8018	0.842	0.8113	0.875	0.8788	0.899	0.6143	0.5018	fold_3
0.5	1.00E-05	0.1	0.01	0.7999	0.822	0.8394	0.8052	0.8745	0.892	0.5964	0.5089	fold_3
0.1	5.00E-06	0	0	0.7897	0.8324	0.8011	0.8663	0.8422	0.8535	0.5902	0.4821	fold_4
0.1	5.00E-06	0	0.01	0.7737	0.8142	0.795	0.8343	0.8369	0.8497	0.553	0.5011	fold_4
0.1	5.00E-06	0.1	0	0.7718	0.813	0.7928	0.8343	0.8425	0.8519	0.5494	0.5347	fold_4
0.1	5.00E-06	0.1	0.01	0.7946	0.8338	0.8087	0.8605	0.8669	0.878	0.5972	0.5011	fold_4
0.1	1.00E-05	0	0	0.7771	0.8295	0.7815	0.8837	0.8387	0.8387	0.5736	0.489	fold_4
0.1	1.00E-05	0	0.01	0.782	0.8247	0.7967	0.8547	0.8415	0.8467	0.573	0.4834	fold_4
0.1	1.00E-05	0.1	0	0.7936	0.8377	0.8011	0.8779	0.8554	0.8596	0.6006	0.5105	fold_4
0.1	1.00E-05	0.1	0.01	0.7883	0.8338	0.7963	0.875	0.8451	0.8601	0.5903	0.5206	fold_4
0.3	5.00E-06	0	0	0.7989	0.8357	0.8149	0.8576	0.8635	0.8758	0.6043	0.4659	fold_4
0.3	5.00E-06	0	0.01	0.7854	0.8275	0.7995	0.8576	0.8449	0.8302	0.5799	0.4876	fold_4
0.3	5.00E-06	0.1	0	0.8028	0.8381	0.8194	0.8576	0.8568	0.8619	0.6113	0.511	fold_4
0.3	5.00E-06	0.1	0.01	0.8125	0.8441	0.831	0.8576	0.8605	0.8778	0.6288	0.5095	fold_4
0.3	1.00E-05	0	0	0.8062	0.8409	0.8222	0.8605	0.8656	0.8793	0.6181	0.4468	fold_4
0.3	1.00E-05	0	0.01	0.7941	0.8312	0.8116	0.8517	0.8625	0.8798	0.5941	0.4663	fold_4
0.3	1.00E-05	0.1	0	0.7994	0.8383	0.812	0.8663	0.8609	0.871	0.6075	0.5102	fold_4

0.3	1.00E-05	0.1	0.01	0.8018	0.839	0.8159	0.8634	0.8643	0.8856	0.611	0.5057	fold_4
0.5	5.00E-06	0	0	0.7825	0.8242	0.7984	0.8517	0.8492	0.8457	0.5731	0.4973	fold_4
0.5	5.00E-06	0	0.01	0.7902	0.835	0.7984	0.875	0.8462	0.856	0.5937	0.4921	fold_4
0.5	5.00E-06	0.1	0	0.7917	0.8336	0.8032	0.8663	0.838	0.8299	0.5936	0.5273	fold_4
0.5	5.00E-06	0.1	0.01	0.7878	0.8282	0.8033	0.8547	0.837	0.8302	0.5834	0.5288	fold_4
0.5	1.00E-05	0	0	0.7878	0.8282	0.8033	0.8547	0.8599	0.8696	0.5834	0.4606	fold_4
0.5	1.00E-05	0	0.01	0.7917	0.821	0.8222	0.8198	0.8616	0.8823	0.5831	0.4683	fold_4
0.5	1.00E-05	0.1	0	0.7776	0.826	0.7868	0.8692	0.8466	0.8659	0.5695	0.527	fold_4
0.5	1.00E-05	0.1	0.01	0.7955	0.8329	0.8122	0.8547	0.8616	0.8782	0.5974	0.517	fold_4
0.1	5.00E-06	0	0	0.8102	0.8336	0.8448	0.8227	0.8783	0.9091	0.6179	0.4405	fold_5
0.1	5.00E-06	0	0.01	0.7985	0.8295	0.8247	0.8343	0.8618	0.8901	0.5982	0.4601	fold_5
0.1	5.00E-06	0.1	0	0.8087	0.8382	0.8333	0.843	0.8739	0.9045	0.6186	0.5027	fold_5
0.1	5.00E-06	0.1	0.01	0.7946	0.8206	0.8304	0.811	0.8654	0.9051	0.5872	0.5156	fold_5
0.1	1.00E-05	0	0	0.7971	0.8213	0.8348	0.8081	0.8664	0.8981	0.5913	0.4605	fold_5
0.1	1.00E-05	0	0.01	0.7834	0.8258	0.7989	0.8547	0.8435	0.86	0.5754	0.5026	fold_5
0.1	1.00E-05	0.1	0	0.7976	0.8174	0.8426	0.7936	0.8632	0.8918	0.5907	0.5054	fold_5
0.1	1.00E-05	0.1	0.01	0.8024	0.8287	0.8348	0.8227	0.8656	0.8973	0.6034	0.5076	fold_5
0.3	5.00E-06	0	0	0.8019	0.8227	0.844	0.8023	0.8722	0.9047	0.5999	0.4511	fold_5
0.3	5.00E-06	0	0.01	0.8014	0.8232	0.8419	0.8052	0.8726	0.9054	0.5992	0.4514	fold_5
0.3	5.00E-06	0.1	0	0.7898	0.8159	0.8269	0.8052	0.8542	0.8811	0.5773	0.5193	fold_5
0.3	5.00E-06	0.1	0.01	0.8019	0.8324	0.8276	0.8372	0.8659	0.8917	0.605	0.5032	fold_5
0.3	1.00E-05	0	0	0.8131	0.8338	0.8515	0.8169	0.8655	0.8904	0.6226	0.4653	fold_5
0.3	1.00E-05	0	0.01	0.8097	0.8372	0.8372	0.8372	0.8814	0.9067	0.6193	0.4523	fold_5
0.3	1.00E-05	0.1	0	0.8092	0.8346	0.8407	0.8285	0.8667	0.8887	0.6169	0.5091	fold_5
0.3	1.00E-05	0.1	0.01	0.8024	0.8287	0.8348	0.8227	0.8719	0.897	0.6034	0.5046	fold_5
0.5	5.00E-06	0	0	0.8087	0.8319	0.8443	0.8198	0.8739	0.9113	0.6148	0.4684	fold_5
0.5	5.00E-06	0	0.01	0.7888	0.8203	0.8179	0.8227	0.8462	0.8598	0.5781	0.4873	fold_5
0.5	5.00E-06	0.1	0	0.8044	0.8267	0.8429	0.811	0.8604	0.8903	0.6054	0.5169	fold_5
0.5	5.00E-06	0.1	0.01	0.7902	0.8187	0.8235	0.814	0.8482	0.8578	0.5794	0.5234	fold_5
0.5	1.00E-05	0	0	0.7946	0.8239	0.8251	0.8227	0.8499	0.8537	0.5889	0.4704	fold_5

0.5	1.00E-05	0	0.01	0.8092	0.8346	0.8407	0.8285	0.864	0.8907	0.6169	0.4485	fold_5
0.5	1.00E-05	0.1	0	0.8024	0.8287	0.8348	0.8227	0.8623	0.8829	0.6034	0.5041	fold_5
0.5	1.00E-05	0.1	0.01	0.7829	0.82	0.8062	0.8343	0.8596	0.8834	0.5697	0.5219	fold_5