Supplementary Material for

Graph Neural Networks in the Nephropathological Diagnosis of Antibody-Mediated Rejection

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S.I. Complete multi-compartment graph classification performance metrics and ROC curves

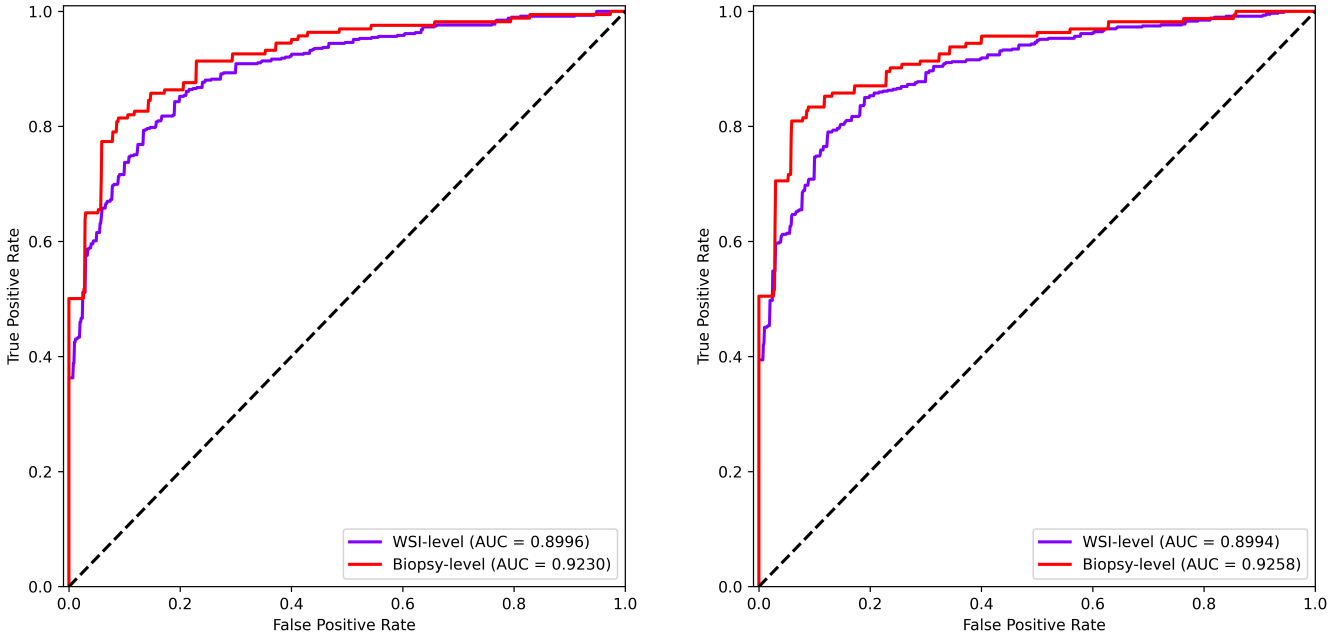
A. Glomeruli + Arteries

			Precision		Sensitivity		Specificity		F1-Score		Balanced accuracy		Accuracy	
Feature extractor	**Classifier**	**k**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**
Swin	Graph-Transformer	1	0.8159	0.8537	0.8339	0.8434	0.7982	0.8644	0.8248	0.8485	0.8160	0.8539	0.8167	0.8542
		2	0.8119	0.8353	0.8559	0.8554	0.7873	0.8418	0.8333	0.8452	0.8216	0.8486	0.8228	0.8484
		3	0.7966	0.8208	0.8627	0.8554	0.7636	0.8249	0.8283	0.8378	0.8132	0.8401	0.8149	0.8397
	SimpleGCN	1	0.8391	0.8580	0.8576	0.8373	0.8236	0.8701	0.8483	0.8476	0.8406	0.8537	0.8412	0.8542
		2	0.8516	0.8688	0.8559	0.8373	0.8400	**0.8814**	0.8538	0.8528	0.8480	0.8594	0.8482	0.8601
		3	**0.8550**	0.8696	**0.8695**	0.8434	0.8418	**0.8814**	**0.8622**	0.8563	**0.8557**	0.8624	**0.8561**	0.8630
	DenseGCN	1	0.8380	0.8625	0.8593	0.8313	0.8218	0.8757	0.8485	0.8466	0.8406	0.8535	0.8412	0.8542
		2	0.8487	0.8580	0.8559	0.8373	0.8364	0.8701	0.8523	0.8476	0.8461	0.8537	0.8465	0.8542
		3	0.8548	0.8712	0.8678	0.8554	0.8418	**0.8814**	0.8612	0.8632	0.8548	0.8684	0.8553	0.8688
	SimpleGAT	1	0.8535	**0.8727**	0.8492	0.8675	**0.8436**	**0.8814**	0.8513	0.8701	0.8464	0.8744	0.8465	**0.8746**
		2	0.8530	0.8589	0.8458	0.8434	**0.8436**	0.8701	0.8494	0.8511	0.8447	0.8567	0.8447	0.8571
		3	0.8454	0.8683	0.8525	**0.8735**	0.8327	0.8757	0.8489	**0.8709**	0.8426	**0.8746**	0.8430	**0.8746**
MAE	Graph-Transformer	1	0.6345	0.6386	0.6356	0.6386	0.6073	0.6610	0.6351	0.6386	0.6214	0.6498	0.6219	0.6501
		2	0.6689	0.6970	0.6780	0.6928	0.6400	0.7175	0.6734	0.6949	0.6590	0.7051	0.6596	0.7055
		3	0.6720	0.6948	0.6356	0.6446	0.6673	0.7345	0.6533	0.6688	0.6514	0.6895	0.6509	0.6910
	SimpleGCN	1	0.6303	0.6481	0.6356	0.6325	0.6000	0.6780	0.6329	0.6402	0.6178	0.6552	0.6184	0.6560
		2	0.6201	0.6306	0.6169	0.5964	0.5945	0.6723	0.6185	0.6130	0.6057	0.6344	0.6061	0.6356
		3	0.6210	0.6203	0.6220	0.5904	0.5927	0.6610	0.6215	0.6049	0.6074	0.6257	0.6079	0.6268
	DenseGCN	1	0.6479	0.6433	0.6424	0.6084	0.6255	0.6836	0.6451	0.6254	0.6339	0.6460	0.6342	0.6472
		2	0.6379	0.6623	0.6271	0.6024	0.6182	0.7119	0.6325	0.6309	0.6227	0.6571	0.6228	0.6589
		3	0.6339	0.6433	0.6339	0.6084	0.6073	0.6836	0.6339	0.6254	0.6206	0.6460	0.6211	0.6472
	SimpleGAT	1	0.6354	0.6646	0.6322	0.6566	0.6109	0.6893	0.6338	0.6606	0.6216	0.6729	0.6219	0.6735
		2	0.6265	0.6415	0.6254	0.6145	0.6000	0.6780	0.6260	0.6277	0.6127	0.6462	0.6132	0.6472
		3	0.6351	0.6415	0.6254	0.6145	0.6145	0.6780	0.6302	0.6277	0.6200	0.6462	0.6202	0.6472
SimCLR	Graph-Transformer	1	0.7082	0.7215	0.6746	0.6867	0.7018	0.7514	0.6910	0.7037	0.6882	0.7191	0.6877	0.7201
		2	0.7082	0.7273	0.7034	0.7229	0.6891	0.7458	0.7058	0.7251	0.6962	0.7343	0.6965	0.7347
		3	0.7031	0.7205	0.6864	0.6988	0.6891	0.7458	0.6947	0.7095	0.6878	0.7223	0.6877	0.7230
	SimpleGCN	1	0.7208	0.7421	0.7000	0.7108	0.7091	0.7684	0.7102	0.7262	0.7045	0.7396	0.7044	0.7405
		2	0.7185	0.7375	0.7051	0.7108	0.7036	0.7627	0.7117	0.7239	0.7044	0.7368	0.7044	0.7376
		3	0.7165	0.7278	0.7153	0.7410	0.6964	0.7401	0.7159	0.7343	0.7058	0.7405	0.7061	0.7405
	DenseGCN	1	0.7095	0.7333	0.7203	0.7289	0.6836	0.7514	0.7149	0.7311	0.7020	0.7402	0.7026	0.7405
		2	0.7243	0.7485	0.7034	0.7349	0.7127	0.7684	0.7137	0.7416	0.7081	0.7517	0.7079	0.7522
		3	0.7051	0.7375	0.6847	0.7108	0.6927	0.7627	0.6948	0.7239	0.6887	0.7368	0.6886	0.7376
	SimpleGAT	1	0.7257	0.7313	0.7220	0.7048	0.7073	0.7571	0.7239	0.7178	0.7147	0.7309	0.7149	0.7318
		2	0.7158	0.7325	0.7000	0.6928	0.7018	0.7627	0.7078	0.7121	0.7009	0.7277	0.7009	0.7289
		3	0.6954	0.7101	0.7119	0.7229	0.6655	0.7232	0.7035	0.7164	0.6887	0.7230	0.6895	0.7230

TABLE S.1 Performance metrics for the test set for hub-based graph (glomeruli + arteries) classification models on the WSIs. Each metric was computed from the aggregated confusion matrix of all 5 test folds, as they are disjoint sets. The best-performing model according to WSI-level accuracy is highlighted in bold, as well as the highest value across models for each metric.

			Precision		Sensitivity		Specificity		F1-Score		Balanced accuracy		Accuracy	
Feature extractor	**Classifier**	α	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**
Swin	Graph-Transformer	0.15	0.8390	0.8742	0.8390	0.8373	0.8273	0.8870	0.8390	0.8554	0.8331	0.8622	0.8333	0.8630
		0.3	0.8195	0.8553	0.8390	0.8193	0.8018	0.8701	0.8291	0.8369	0.8204	0.8447	0.8211	0.8455
		0.5	0.8260	0.8590	0.8288	0.8072	0.8127	0.8757	0.8274	0.8323	0.8208	0.8415	0.8211	0.8426
	SimpleGCN	0.15	0.8399	0.8704	0.8627	0.8494	0.8236	0.8814	0.8512	0.8598	0.8432	0.8654	0.8439	0.8659
		0.3	0.8374	0.8780	0.8729	**0.8675**	0.8182	0.8870	0.8548	**0.8727**	0.8455	**0.8772**	0.8465	**0.8776**
		0.5	**0.8467**	0.8720	**0.8797**	0.8614	**0.8291**	0.8814	**0.8628**	0.8667	**0.8544**	0.8714	**0.8553**	0.8717
	DenseGCN	0.15	0.8325	0.8528	0.8508	0.8373	0.8164	0.8644	0.8416	0.8450	0.8336	0.8509	0.8342	0.8513
		0.3	0.8382	0.8659	0.8695	0.8554	0.8200	0.8757	0.8536	0.8606	0.8447	0.8656	0.8456	0.8659
		0.5	0.8438	**0.8820**	0.8695	0.8554	0.8273	**0.8927**	0.8564	0.8685	0.8484	0.8740	0.8491	0.8746
MAE	Graph-Transformer	0.15	0.6750	0.7000	0.6407	0.6747	0.6691	0.7288	0.6574	0.6871	0.6549	0.7018	0.6544	0.7026
		0.3	0.6760	0.7059	0.6542	0.6506	0.6636	0.7458	0.6649	0.6771	0.6589	0.6982	0.6588	0.6997
		0.5	0.6490	0.6772	0.6424	0.6446	0.6273	0.7119	0.6457	0.6605	0.6348	0.6782	0.6351	0.6793
	SimpleGCN	0.15	0.6401	0.6581	0.6390	0.6145	0.6145	0.7006	0.6395	0.6355	0.6268	0.6575	0.6272	0.6589
		0.3	0.6250	0.6316	0.6441	0.6506	0.5855	0.6441	0.6344	0.6409	0.6148	0.6473	0.6158	0.6472
		0.5	0.6130	0.6433	0.6068	0.6084	0.5891	0.6836	0.6099	0.6254	0.5979	0.6460	0.5982	0.6472
	DenseGCN	0.15	0.6282	0.6494	0.6186	0.6024	0.6073	0.6949	0.6234	0.6250	0.6130	0.6487	0.6132	0.6501
		0.3	0.6081	0.6380	0.6339	0.6265	0.5618	0.6667	0.6207	0.6322	0.5979	0.6466	0.5991	0.6472
		0.5	0.6432	0.6623	0.6051	0.6024	0.6400	0.7119	0.6236	0.6309	0.6225	0.6571	0.6219	0.6589
SimCLR	Graph-Transformer	0.15	0.7173	0.7677	0.6881	0.7169	0.7091	0.7966	0.7024	0.7414	0.6986	0.7567	0.6982	0.7580
		0.3	0.7113	0.7346	0.6847	0.7169	0.7018	0.7571	0.6978	0.7256	0.6933	0.7370	0.6930	0.7376
		0.5	0.7163	0.7516	0.6932	0.6928	0.7055	0.7853	0.7046	0.7210	0.6993	0.7390	0.6991	0.7405
	SimpleGCN	0.15	0.7012	0.7246	0.6881	0.7289	0.6855	0.7401	0.6946	0.7267	0.6868	0.7345	0.6868	0.7347
		0.3	0.6965	0.7246	0.7000	0.7289	0.6727	0.7401	0.6982	0.7267	0.6864	0.7345	0.6868	0.7347
		0.5	0.7075	0.7229	0.7051	0.7229	0.6873	0.7401	0.7063	0.7229	0.6962	0.7315	0.6965	0.7318
	DenseGCN	0.15	0.7180	0.7405	0.7034	0.7048	0.7036	0.7684	0.7106	0.7222	0.7035	0.7366	0.7035	0.7376
		0.3	0.7070	0.7284	0.7034	0.7108	0.6873	0.7514	0.7052	0.7195	0.6953	0.7311	0.6956	0.7318
		0.5	0.7101	0.7452	0.7017	0.7048	0.6927	0.7740	0.7059	0.7245	0.6972	0.7394	0.6974	0.7405

TABLE S.2 Performance metrics for the test set for edge-weighted graph (glomeruli + arteries) classification models on the WSIs. Each metric was computed from the aggregated confusion matrix of all 5 test folds, as they are disjoint sets. The best-performing model according to WSI-level accuracy is highlighted in bold, as well as the highest value across models for each metric.



(a) Hub-based

(b) Edge-weighted

Fig. S.1. ROC curve and average AUC on the test set of the WSIs across 5 folds for the best-performing graph (glomeruli + arteries) classification model configuration with each graph construction approach.

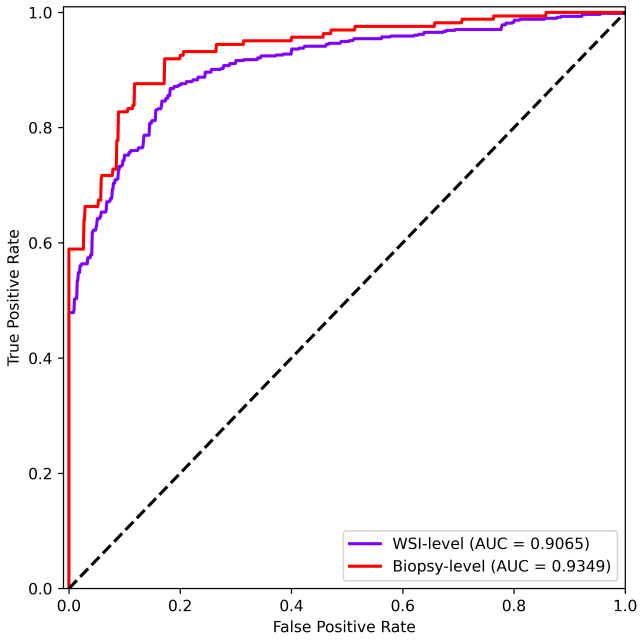
B. Glomeruli + Cortical TI tiles

			Precision		Sensitivity		Specificity		F1-Score		Balanced accuracy		Accuracy	
Feature extractor	**Classifier**	**k**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**
Swin	Graph-Transformer	1	0.8272	0.8402	0.8342	0.8503	0.8123	0.8475	0.8307	0.8452	0.8232	0.8489	0.8236	0.8488
		2	0.8264	0.8563	0.8291	0.8563	0.8123	0.8644	0.8278	0.8563	0.8207	0.8603	0.8210	0.8605
		3	0.8342	0.8623	0.8342	0.8623	0.8213	0.8701	0.8342	0.8623	0.8277	0.8662	0.8280	0.8663
	SimpleGCN	1	0.8522	0.8743	0.8693	0.8743	0.8375	0.8814	0.8607	0.8743	0.8534	0.8778	0.8540	0.8779
		2	0.8607	0.8788	0.8693	0.8683	0.8484	0.8870	0.8650	0.8735	**0.8589**	0.8776	**0.8593**	0.8779
		3	0.8499	0.8757	0.8727	0.8862	0.8339	0.8814	0.8612	0.8810	0.8533	0.8838	0.8540	0.8837
	DenseGCN	1	0.8435	0.8614	0.8576	0.8563	0.8285	0.8701	0.8505	0.8589	0.8431	0.8632	0.8436	0.8634
		2	0.8449	0.8596	0.8576	0.8802	0.8303	0.8644	0.8512	0.8698	0.8440	0.8723	0.8445	0.8721
		3	0.8550	0.8667	0.8593	0.8563	0.8430	0.8757	0.8571	0.8614	0.8511	0.8660	0.8514	0.8663
	SimpleGAT	1	0.8500	0.8772	**0.8827**	**0.8982**	0.8321	0.8814	**0.8661**	0.8876	0.8574	0.8898	0.8584	0.8895
		2	0.8476	0.8671	0.8760	**0.8982**	0.8303	0.8701	0.8616	0.8824	0.8532	0.8841	0.8540	0.8837
		3	**0.8653**	**0.8916**	0.8610	0.8862	**0.8556**	**0.8983**	0.8631	**0.8889**	0.8583	**0.8923**	0.8584	**0.8924**
MAE	Graph-Transformer	1	0.6465	0.6471	0.5913	0.5928	0.6516	0.6949	0.6177	0.6188	0.6215	0.6439	0.6203	0.6453
		2	0.6838	0.6968	0.6449	0.6467	0.6787	0.7345	0.6638	0.6708	0.6618	0.6906	0.6612	0.6919
		3	0.6808	0.6774	0.6466	0.6287	0.6733	0.7175	0.6632	0.6522	0.6599	0.6731	0.6594	0.6744
	SimpleGCN	1	0.6070	0.6243	0.6415	0.6467	0.5523	0.6328	0.6238	0.6353	0.5969	0.6397	0.5986	0.6395
		2	0.6042	0.6364	0.6214	0.6287	0.5614	0.6610	0.6127	0.6325	0.5914	0.6449	0.5925	0.6453
		3	0.6091	0.6358	0.6499	0.6587	0.5505	0.6441	0.6288	0.6471	0.6002	0.6514	0.6021	0.6512
	DenseGCN	1	0.6182	0.6159	0.6482	0.6048	0.5686	0.6441	0.6329	0.6103	0.6084	0.6244	0.6099	0.6250
		2	0.6013	0.6289	0.6064	0.5988	0.5668	0.6667	0.6038	0.6135	0.5866	0.6327	0.5873	0.6337
		3	0.6211	0.6410	0.6315	0.5988	0.5848	0.6836	0.6262	0.6192	0.6082	0.6412	0.6090	0.6424
	SimpleGAT	1	0.6127	0.6433	0.6147	0.6048	0.5812	0.6836	0.6137	0.6235	0.5980	0.6442	0.5986	0.6453
		2	0.6190	0.6688	0.6231	0.6287	0.5866	0.7062	0.6210	0.6481	0.6049	0.6675	0.6056	0.6686
		3	0.6038	0.6296	0.5846	0.6108	0.5866	0.6610	0.5940	0.6201	0.5856	0.6359	0.5856	0.6366
SimCLR	Graph-Transformer	1	0.7325	0.7375	0.6834	0.7066	0.7310	0.7627	0.7071	0.7217	0.7072	0.7346	0.7063	0.7355
		2	0.7140	0.7389	0.6734	0.6946	0.7094	0.7684	0.6931	0.7160	0.6914	0.7315	0.6907	0.7326
		3	0.7082	0.7152	0.6951	0.6766	0.6913	0.7458	0.7016	0.6954	0.6932	0.7112	0.6933	0.7122
	SimpleGCN	1	0.7416	0.7605	0.7353	0.7605	0.7238	0.7740	0.7384	0.7605	0.7296	0.7672	0.7298	0.7674
		2	0.7547	0.7673	0.7320	0.7305	0.7437	0.7910	0.7432	0.7485	0.7378	0.7607	0.7376	0.7616
		3	0.7414	0.7799	0.7253	0.7425	0.7274	0.8023	0.7333	0.7607	0.7264	0.7724	0.7263	0.7733
	DenseGCN	1	0.7325	0.7702	0.7203	0.7425	0.7166	0.7910	0.7264	0.7561	0.7184	0.7667	0.7185	0.7674
		2	0.7337	0.7607	0.7337	0.7425	0.7130	0.7797	0.7337	0.7515	0.7233	0.7611	0.7237	0.7616
		3	0.7356	0.7688	0.7270	0.7365	0.7184	0.7910	0.7313	0.7523	0.7227	0.7637	0.7228	0.7645
	SimpleGAT	1	0.7317	0.7410	0.7219	0.7365	0.7148	0.7571	0.7268	0.7387	0.7184	0.7468	0.7185	0.7471
		2	0.7402	0.7622	0.7253	0.7485	0.7256	0.7797	0.7327	0.7553	0.7255	0.7641	0.7255	0.7645
		3	0.7300	0.7396	0.7337	0.7485	0.7076	0.7514	0.7318	0.7440	0.7206	0.7500	0.7211	0.7500

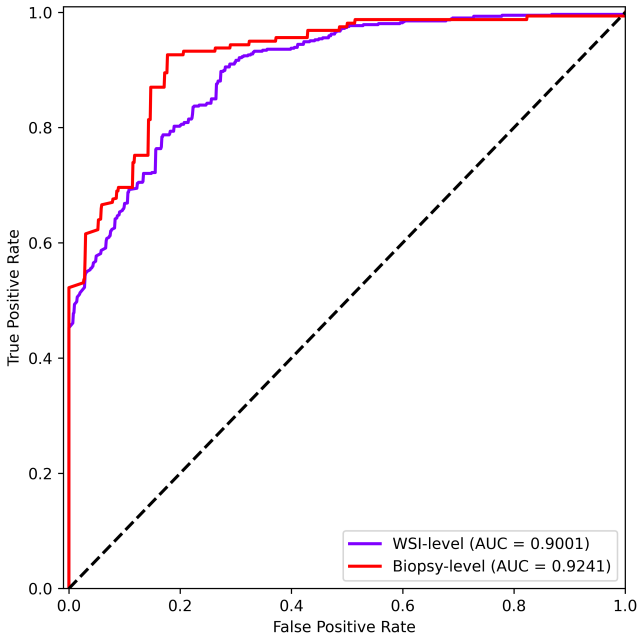
TABLE S.3 Performance metrics for the test set for hub-based graph (glomeruli + cortical TI tiles) classification models on the WSIs. Each metric was computed from the aggregated confusion matrix of all 5 test folds, as they are disjoint sets. The best-performing model according to WSI-level accuracy is highlighted in bold, as well as the highest value across models for each metric.

			Precision		Sensitivity		Specificity		F1-Score		Balanced accuracy		Accuracy	
Feature extractor	**Classifier**	α	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**
Swin	Graph-Transformer	0.15	0.8537	0.8773	0.8308	0.8563	0.8466	0.8870	0.8421	0.8667	0.8387	0.8716	0.8384	0.8721
		0.3	0.8559	0.8647	0.8358	0.8802	0.8484	0.8701	0.8458	0.8724	0.8421	0.8751	0.8419	0.8750
		0.5	0.8463	0.8712	0.8392	0.8503	0.8357	0.8814	0.8427	0.8606	0.8375	0.8658	0.8375	0.8663
	SimpleGCN	0.15	**0.8697**	0.8889	0.8610	0.8623	**0.8610**	0.8983	0.8653	0.8754	0.8610	0.8803	0.8610	0.8808
		0.3	0.8636	0.8909	0.8693	0.8802	0.8520	0.8983	0.8664	0.8855	0.8607	0.8893	0.8610	0.8895
		0.5	0.8661	**0.8951**	0.8559	0.8683	0.8574	**0.9040**	0.8610	0.8815	0.8567	0.8861	0.8566	0.8866
	DenseGCN	0.15	0.8634	0.8795	0.8576	0.8743	0.8538	0.8870	0.8605	0.8769	0.8557	0.8806	0.8558	0.8808
		0.3	0.8682	0.8830	**0.8827**	**0.9042**	0.8556	0.8870	**0.8754**	**0.8935**	**0.8692**	**0.8956**	**0.8697**	**0.8953**
		0.5	0.8506	0.8596	0.8677	0.8802	0.8357	0.8644	0.8590	0.8698	0.8517	0.8723	0.8523	0.8721
MAE	Graph-Transformer	0.15	0.6394	0.6689	0.6030	0.5928	0.6336	0.7232	0.6207	0.6286	0.6183	0.6580	0.6177	0.6599
		0.3	0.6087	0.6207	0.6332	0.6467	0.5614	0.6271	0.6207	0.6334	0.5973	0.6369	0.5986	0.6366
		0.5	0.6094	0.6129	0.5879	0.5689	0.5939	0.6610	0.5985	0.5901	0.5909	0.6149	0.5908	0.6163
	SimpleGCN	0.15	0.6079	0.6287	0.6415	0.6287	0.5542	0.6497	0.6243	0.6287	0.5978	0.6392	0.5995	0.6395
		0.3	0.6015	0.6215	0.6549	0.6587	0.5325	0.6215	0.6271	0.6395	0.5937	0.6401	0.5960	0.6395
		0.5	0.6069	0.6273	0.6231	0.6048	0.5650	0.6610	0.6149	0.6159	0.5940	0.6329	0.5951	0.6337
	DenseGCN	0.15	0.6003	0.6194	0.5863	0.5749	0.5794	0.6667	0.5932	0.5963	0.5828	0.6208	0.5830	0.6221
		0.3	0.6010	0.6145	0.6332	0.6108	0.5469	0.6384	0.6166	0.6126	0.5900	0.6246	0.5917	0.6250
		0.5	0.5967	0.5951	0.6047	0.5808	0.5596	0.6271	0.6007	0.5879	0.5821	0.6040	0.5830	0.6047
SimCLR	Graph-Transformer	0.15	0.7327	0.7415	0.6566	0.6527	0.7419	0.7853	0.6926	0.6943	0.6992	0.7190	0.6977	0.7209
		0.3	0.7303	0.7432	0.6533	0.6587	0.7401	0.7853	0.6897	0.6984	0.6967	0.7220	0.6950	0.7238
		0.5	0.7331	0.7578	0.7085	0.7305	0.7220	0.7797	0.7206	0.7439	0.7153	0.7551	0.7150	0.7558
	SimpleGCN	0.15	0.7436	0.7563	0.7286	0.7246	0.7292	0.7797	0.7360	0.7401	0.7289	0.7521	0.7289	0.7529
		0.3	0.7387	0.7673	0.7387	0.7305	0.7184	0.7910	0.7387	0.7485	0.7286	0.7607	0.7289	0.7616
		0.5	0.7286	0.7531	0.7286	0.7305	0.7076	0.7740	0.7286	0.7416	0.7181	0.7523	0.7185	0.7529
	DenseGCN	0.15	0.7174	0.7333	0.7102	0.7246	0.6986	0.7514	0.7138	0.7289	0.7044	0.7380	0.7046	0.7384
		0.3	0.7268	0.7515	0.7219	0.7425	0.7076	0.7684	0.7244	0.7470	0.7148	0.7554	0.7150	0.7558
		0.5	0.7131	0.7301	0.6951	0.7126	0.6986	0.7514	0.7040	0.7212	0.6968	0.7320	0.6968	0.7326

TABLE S.4 Performance metrics for the test set for edge-weighted graph (glomeruli + cortical TI tiles) classification models on the WSIs. Each metric was computed from the aggregated confusion matrix of all 5 test folds, as they are disjoint sets. The best-performing model according to WSI-level accuracy is highlighted in bold, as well as the highest value across models for each metric.



(a) Hub-based



(b) Edge-weighted

Fig. S.2. ROC curve and average AUC on the test set of the WSIs across 5 folds for the best-performing graph (glomeruli + cortical TI tiles) classification model configuration with each graph construction approach.

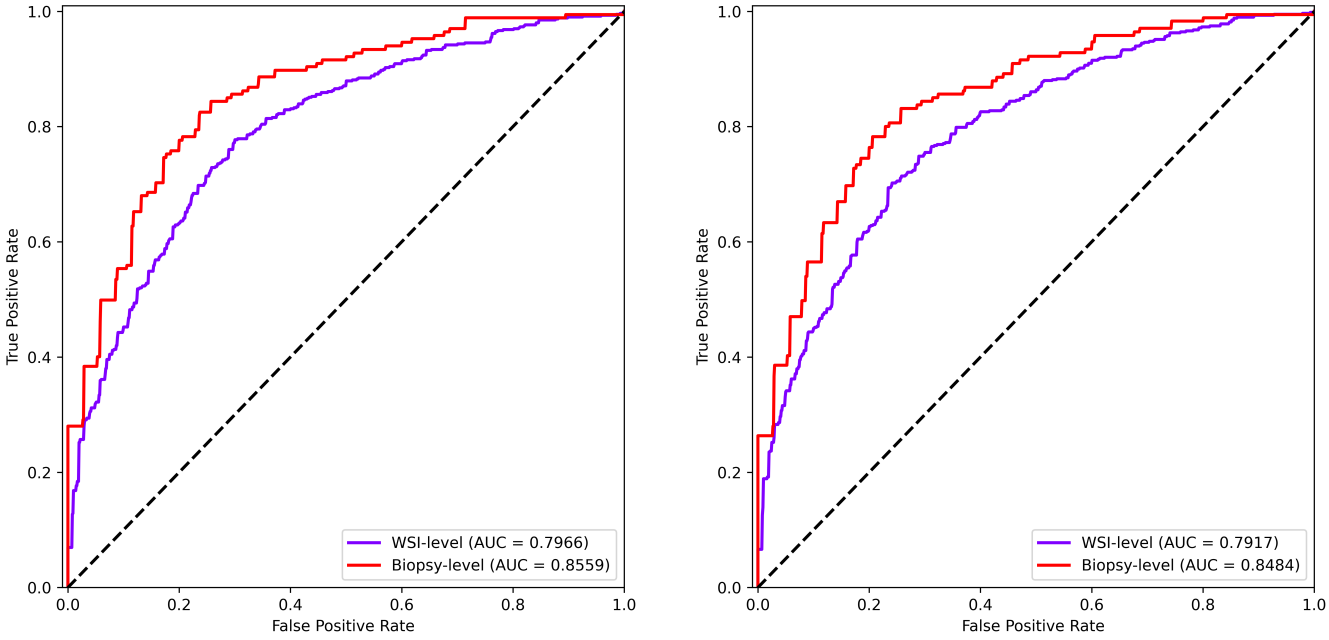
C. Glomeruli + Arteries + Cortical TI tiles

			Precision		Sensitivity		Specificity		F1-Score		Balanced accuracy		Accuracy	
Feature extractor	**Classifier**	**k**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**
Swin	Graph-Transformer	1	0.6990	0.7176	0.7188	0.7305	0.6643	0.7288	0.7088	0.7240	0.6915	0.7297	0.6926	0.7297
		2	0.6883	0.7072	0.7238	0.7665	0.6444	0.7006	0.7056	0.7356	0.6841	0.7335	0.6857	0.7326
		3	0.6868	0.7039	0.7371	0.7545	0.6354	0.7006	0.7111	0.7283	0.6862	0.7275	0.6883	0.7267
	SimpleGCN	1	0.6724	0.6837	**0.7854**	0.8024	0.5848	0.6497	0.7245	0.7383	0.6851	0.7261	0.6892	0.7238
		2	0.6749	0.7016	0.7704	0.8024	0.5975	0.6780	0.7195	0.7486	0.6839	0.7402	0.6874	0.7384
		3	0.6710	0.7021	0.7704	0.7904	0.5903	0.6836	0.7173	0.7437	0.6803	0.7370	0.6840	0.7355
	DenseGCN	1	0.6739	0.6989	0.7704	0.7784	0.5957	0.6836	0.7189	0.7365	0.6830	0.7310	0.6866	0.7297
		2	0.6799	0.7120	0.7671	0.7844	0.6083	0.7006	0.7209	0.7464	0.6877	0.7425	0.6909	0.7413
		3	0.6799	0.7059	0.7704	0.7904	0.6065	0.6893	0.7223	0.7458	0.6884	0.7398	0.6918	0.7384
	SimpleGAT	1	0.6778	0.6979	0.7770	0.8024	0.5993	0.6723	0.7240	0.7465	0.6882	0.7374	0.6918	0.7355
		2	0.6709	0.6935	0.7837	**0.8263**	0.5830	0.6554	0.7229	0.7541	0.6834	0.7409	0.6874	0.7384
		3	0.6815	0.6952	0.7621	0.7784	0.6137	0.6780	0.7196	0.7345	0.6879	0.7282	0.6909	0.7267
MAE	Graph-Transformer	1	0.6513	0.6646	0.6123	0.6287	0.6444	0.7006	0.6312	0.6462	0.6284	0.6647	0.6277	0.6657
		2	0.6580	0.6731	0.6339	0.6287	0.6426	0.7119	0.6458	0.6502	0.6383	0.6703	0.6381	0.6715
		3	0.6632	0.6774	0.6423	0.6287	0.6462	0.7175	0.6526	0.6522	0.6442	0.6731	0.6442	0.6744
	SimpleGCN	1	0.5808	0.6199	0.6156	0.6347	0.5181	0.6328	0.5977	0.6272	0.5668	0.6337	0.5688	0.6337
		2	0.6010	0.6242	0.5840	0.5868	0.5794	0.6667	0.5924	0.6049	0.5817	0.6267	0.5818	0.6279
		3	0.5867	0.5943	0.6473	0.6228	0.5054	0.5989	0.6155	0.6082	0.5763	0.6108	0.5792	0.6105
	DenseGCN	1	0.5821	0.5890	0.6073	0.5749	0.5271	0.6215	0.5945	0.5818	0.5672	0.5982	0.5688	0.5988
		2	0.5997	0.6257	0.6506	0.6407	0.5289	0.6384	0.6241	0.6331	0.5897	0.6396	0.5922	0.6395
		3	0.5909	0.5976	0.6273	0.5868	0.5289	0.6271	0.6086	0.5921	0.5781	0.6070	0.5801	0.6076
	SimpleGAT	1	0.6117	0.6460	0.6290	0.6228	0.5668	0.6780	0.6202	0.6341	0.5979	0.6504	0.5991	0.6512
		2	0.6165	0.6456	0.6206	0.6108	0.5812	0.6836	0.6186	0.6277	0.6009	0.6472	0.6017	0.6483
		3	0.6100	0.6585	0.6090	0.6467	0.5776	0.6836	0.6095	0.6526	0.5933	0.6652	0.5939	0.6657
SimCLR	Graph-Transformer	1	0.7097	0.7296	0.7038	0.6946	0.6877	0.7571	0.7068	0.7117	0.6958	0.7258	0.6961	0.7267
		2	0.7219	0.7500	0.6522	0.6826	**0.7274**	0.7853	0.6853	0.7147	0.6898	0.7340	0.6883	0.7355
		3	0.7152	0.7515	0.7188	0.7425	0.6895	0.7684	0.7170	0.7470	0.7042	0.7554	0.7048	0.7558
	SimpleGCN	1	0.7409	0.7764	0.7421	0.7485	0.7184	**0.7966**	0.7415	0.7622	0.7303	0.7726	0.7307	0.7733
		2	**0.7441**	0.7744	0.7404	0.7605	0.7238	0.7910	**0.7423**	0.7674	**0.7321**	0.7757	**0.7325**	0.7762
		3	0.7429	**0.7818**	0.7404	0.7725	0.7220	**0.7966**	0.7417	**0.7771**	0.7312	**0.7845**	0.7316	**0.7849**
	DenseGCN	1	0.7262	0.7391	0.7371	0.7126	0.6986	0.7627	0.7316	0.7256	0.7178	0.7376	0.7186	0.7384
		2	0.7347	0.7391	0.7188	0.7126	0.7184	0.7627	0.7267	0.7256	0.7186	0.7376	0.7186	0.7384
		3	0.7243	0.7412	0.7388	0.7545	0.6949	0.7514	0.7315	0.7478	0.7169	0.7530	0.7177	0.7529
	SimpleGAT	1	0.7265	0.7654	0.7205	0.7425	0.7058	0.7853	0.7235	0.7538	0.7131	0.7639	0.7134	0.7645
		2	0.7298	0.7607	0.7371	0.7425	0.7040	0.7797	0.7334	0.7515	0.7205	0.7611	0.7212	0.7616
		3	0.7294	0.7500	0.7354	0.7365	0.7040	0.7684	0.7324	0.7432	0.7197	0.7524	0.7203	0.7529

TABLE S.5 Performance metrics for the test set for hub-based graph (glomeruli + arteries + cortical TI tiles) classification models on the WSIs. Each metric was computed from the aggregated confusion matrix of all 5 test folds, as they are disjoint sets. The best-performing model according to WSI-level accuracy is highlighted in bold, as well as the highest value across models for each metric.

			Precision		Sensitivity		Specificity		F1-Score		Balanced accuracy		Accuracy	
Feature extractor	**Classifier**	α	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**	**WSI-level**	**Biopsy-level**
Swin	Graph-Transformer	0.15	0.6874	0.6957	0.7537	0.7665	0.6282	0.6836	0.7190	0.7293	0.6910	0.7250	0.6935	0.7238
		0.3	0.6882	0.7151	0.7637	0.7665	0.6245	0.7119	0.7240	0.7399	0.6941	0.7392	0.6970	0.7384
		0.5	0.6785	0.6811	0.7654	0.7545	0.6065	0.6667	0.7193	0.7159	0.6859	0.7106	0.6892	0.7093
	SimpleGCN	0.15	0.6696	0.6935	0.7587	0.7725	0.5939	0.6780	0.7114	0.7309	0.6763	0.7252	0.6797	0.7238
		0.3	0.6706	0.6923	0.7554	0.7545	0.5975	0.6836	0.7105	0.7221	0.6764	0.7191	0.6797	0.7180
		0.5	0.6681	0.6919	0.7637	0.7665	0.5884	0.6780	0.7127	0.7273	0.6761	0.7222	0.6797	0.7209
	DenseGCN	0.15	0.6734	0.7090	**0.7754**	**0.8024**	0.5921	0.6893	0.7208	0.7528	0.6837	0.7458	0.6874	0.7442
		0.3	0.6760	0.7027	0.7671	0.7784	0.6011	0.6893	0.7186	0.7386	0.6841	0.7339	0.6874	0.7326
		0.5	0.6779	0.7021	0.7704	0.7904	0.6029	0.6836	0.7212	0.7437	0.6866	0.7370	0.6900	0.7355
MAE	Graph-Transformer	0.15	0.6254	0.6282	0.6140	0.5868	0.6011	0.6723	0.6196	0.6068	0.6075	0.6296	0.6078	0.6308
		0.3	0.6043	0.6108	0.6023	0.6108	0.5722	0.6328	0.6033	0.6108	0.5873	0.6218	0.5879	0.6221
		0.5	0.6096	0.6205	0.6106	0.6168	0.5758	0.6441	0.6101	0.6186	0.5932	0.6304	0.5939	0.6308
	SimpleGCN	0.15	0.5945	0.6296	0.6073	0.6108	0.5505	0.6610	0.6008	0.6201	0.5789	0.6359	0.5801	0.6366
		0.3	0.5746	0.5965	0.6090	0.6108	0.5108	0.6102	0.5913	0.6036	0.5599	0.6105	0.5619	0.6105
		0.5	0.5792	0.5989	0.6206	0.6347	0.5108	0.5989	0.5992	0.6163	0.5657	0.6168	0.5680	0.6163
	DenseGCN	0.15	0.6000	0.6221	0.6439	0.6407	0.5343	0.6328	0.6212	0.6313	0.5891	0.6367	0.5913	0.6366
		0.3	0.5898	0.6319	0.5957	0.6168	0.5505	0.6610	0.5927	0.6242	0.5731	0.6389	0.5740	0.6395
		0.5	0.5990	0.6273	0.6140	0.6048	0.5542	0.6610	0.6064	0.6159	0.5841	0.6329	0.5853	0.6337
SimCLR	Graph-Transformer	0.15	0.7314	0.7547	0.7022	0.7186	0.7202	0.7797	0.7165	0.7362	0.7112	0.7491	0.7108	0.7500
		0.3	0.7138	0.7197	0.6722	0.6766	0.7076	0.7514	0.6924	0.6975	0.6899	0.7140	0.6892	0.7151
		0.5	0.7237	0.7134	0.6755	0.7006	0.7202	0.7345	0.6988	0.7069	0.6979	0.7175	0.6970	0.7180
	SimpleGCN	**0.15**	0.7405	0.7619	0.7454	0.7665	0.7166	0.7740	**0.7430**	0.7642	**0.7310**	0.7702	**0.7316**	0.7703
		0.3	0.7399	**0.7785**	0.7288	0.7365	0.7220	**0.8023**	0.7343	0.7569	0.7254	0.7694	0.7255	0.7703
		0.5	**0.7458**	0.7711	0.7321	0.7665	**0.7292**	0.7853	0.7389	**0.7688**	0.7307	**0.7759**	0.7307	**0.7762**
	DenseGCN	0.15	0.7152	0.7394	0.7354	0.7305	0.6823	0.7571	0.7252	0.7349	0.7089	0.7438	0.7100	0.7442
		0.3	0.7033	0.7440	0.7338	0.7485	0.6643	0.7571	0.7182	0.7463	0.6990	0.7528	0.7004	0.7529
		0.5	0.7169	0.7381	0.7205	0.7425	0.6913	0.7514	0.7187	0.7403	0.7059	0.7470	0.7065	0.7471

TABLE S.6 Performance metrics for the test set for edge-weighted graph (glomeruli + arteries + cortical TI tiles) classification models on the WSIs. Each metric was computed from the aggregated confusion matrix of all 5 test folds, as they are disjoint sets. The best-performing model according to WSI-level accuracy is highlighted in bold, as well as the highest value across models for each metric.



(a) Hub-based

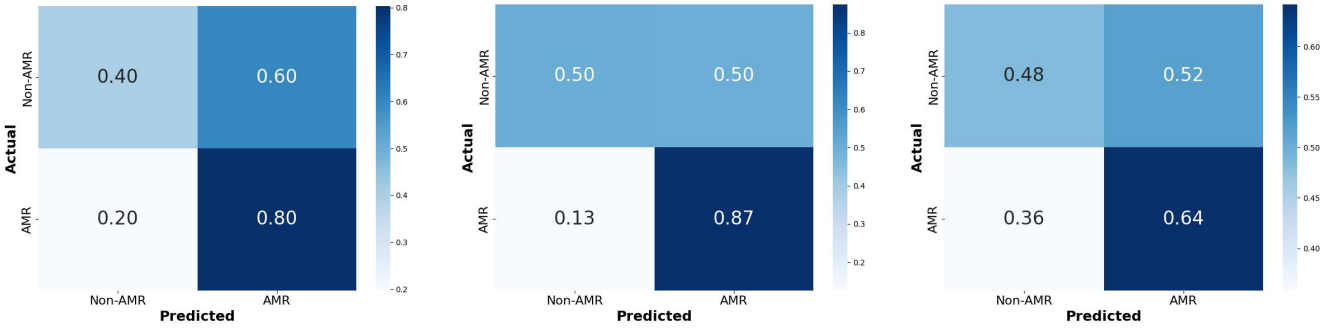
(b) Edge-weighted

Fig. S.3. ROC curve and average AUC on the test set of the WSIs across 5 folds for the best-performing graph (glomeruli + arteries + cortical TI tiles) classification model configuration with each graph construction approach.

S.II. Aggregated confusion matrices

A. Mini-dataset

1) Baseline classification models



(a) ConvNeXt (b) Swin (c) EfficientNet

Fig. S.4. Normalized confusion matrices for the test set for baseline classification models on the mini-dataset. The confusion matrices of all 5 test folds were aggregated and normalized.

2) Graph classification models

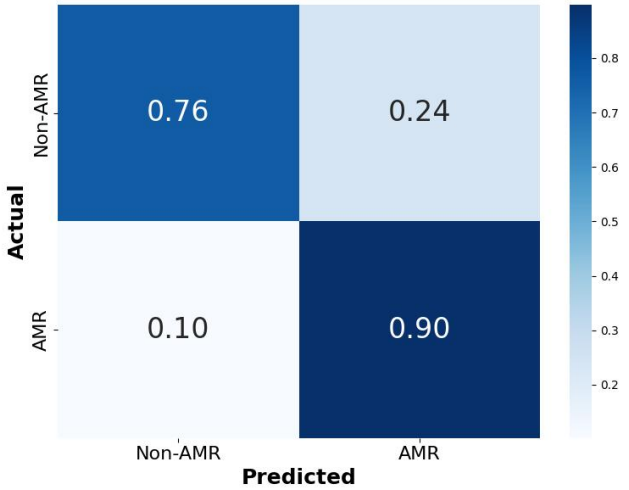
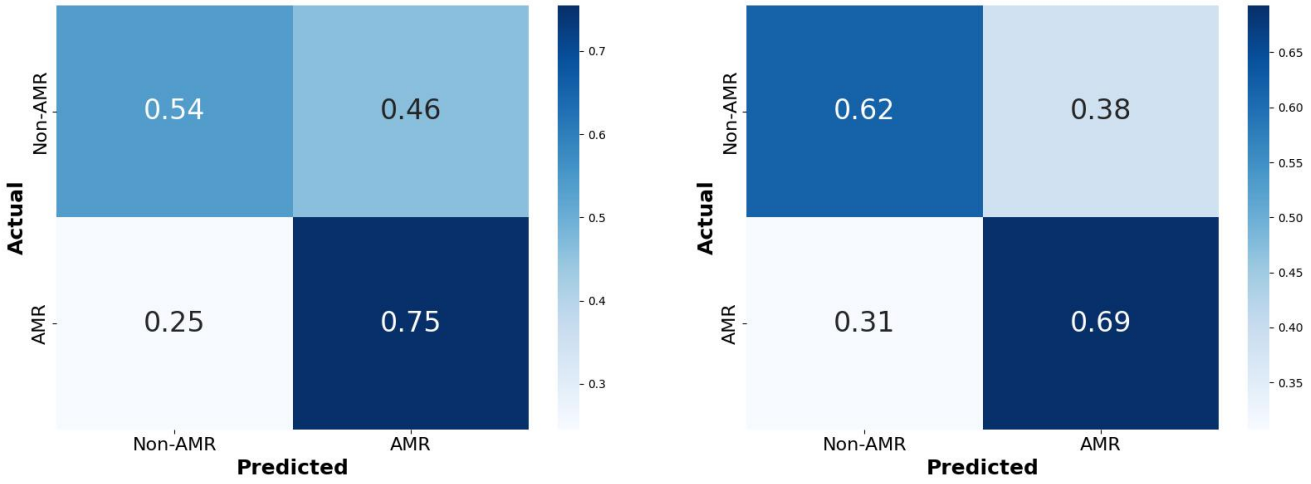


Fig. S.5. Normalized confusion matrices on the test set of the mini-dataset for the best-performing graph classification model, Graph-Transformer using MAE as feature extractor to construct the graphs. The confusion matrices of all 5 test folds were aggregated and normalized.

B. WSIs

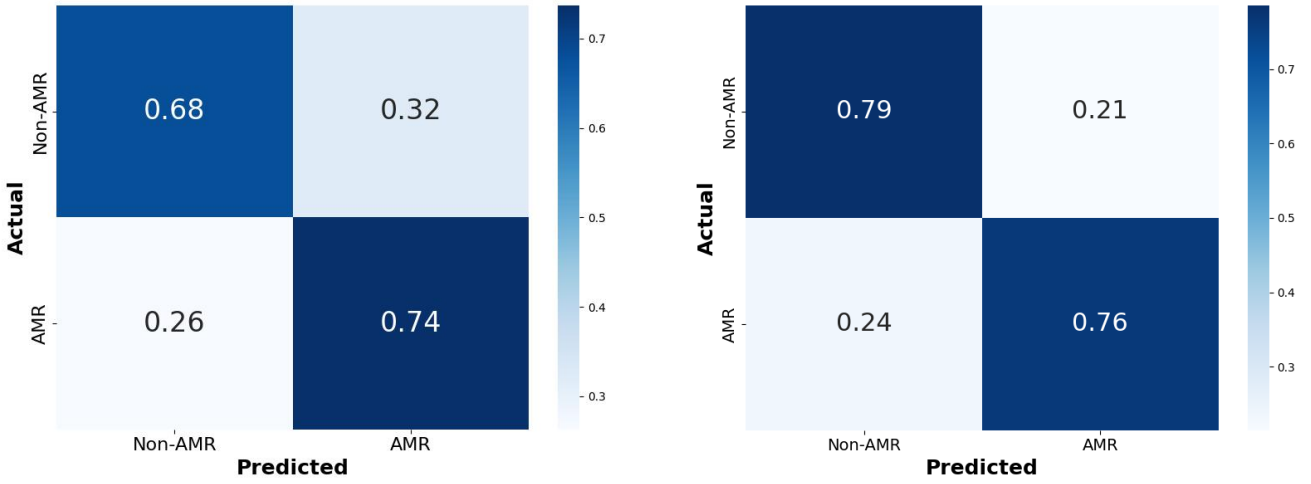
1) Baseline classification models



(a) ConvNeXt (b) Swin

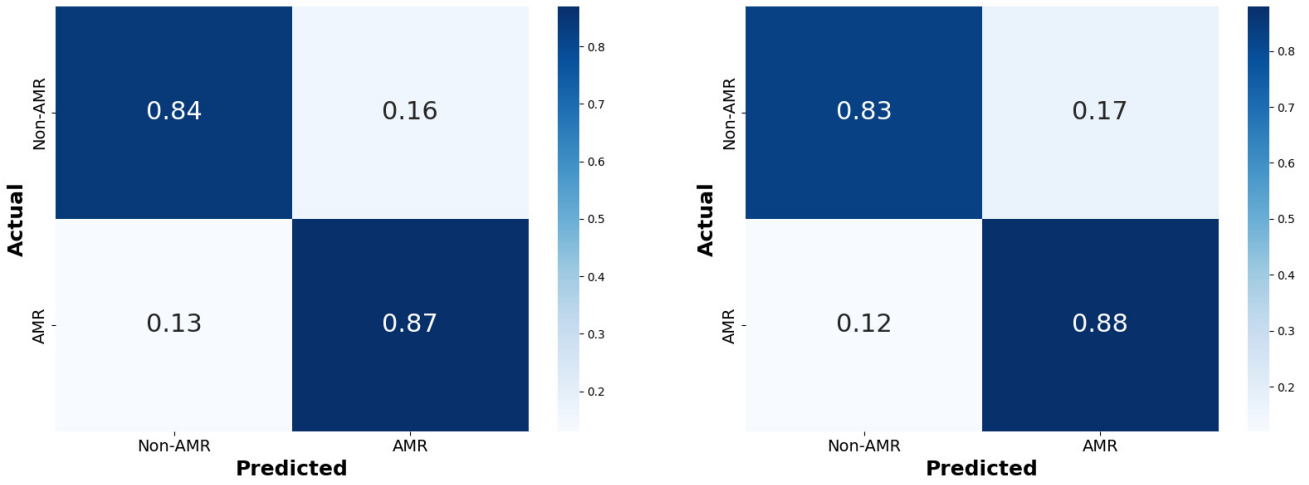
Fig. S.6. Normalized confusion matrices on the test set for baseline classification models on the WSIs. The confusion matrices of all 5 test folds were aggregated and normalized.

2) Graph classification models



(a) WSI-level (b) Biopsy-level

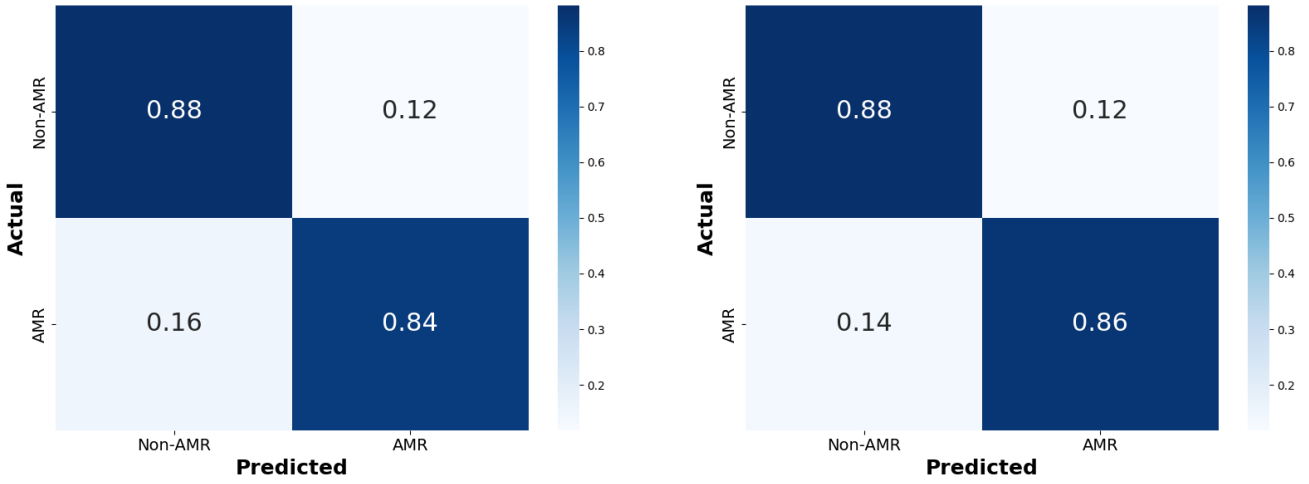
Fig. S.7. Normalized confusion matrix on the test set of the WSIs for the best-performing glomeruli-only graph classification model, SimpleGCN using Swin as feature extractor to construct the graphs. The confusion matrices of all 5 test folds were aggregated and normalized.



(a) Hub-based

(b) Edge-weighted

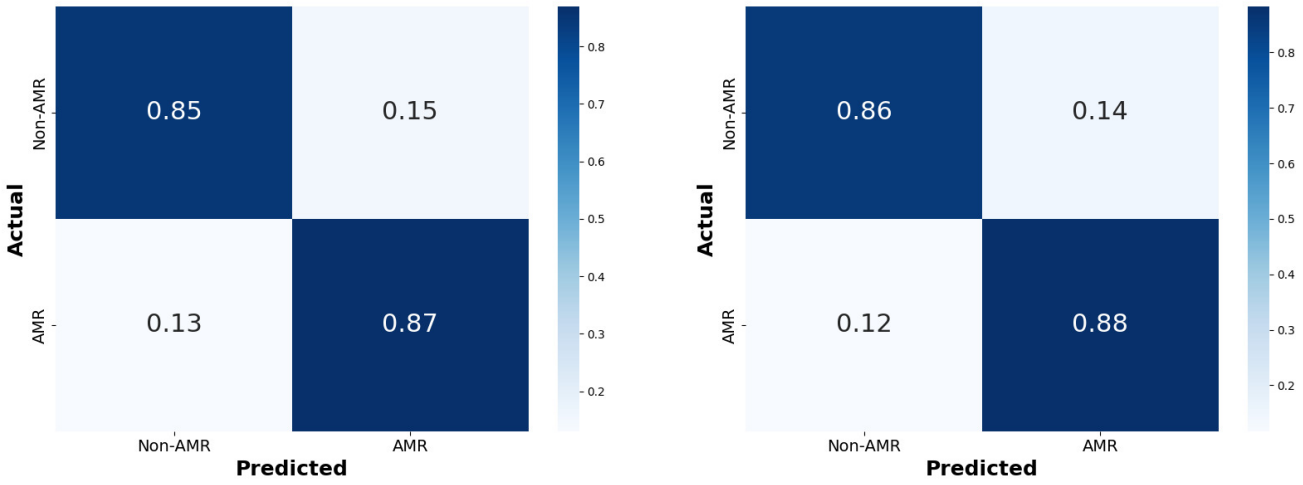
Fig. S.8. Normalized confusion matrix on the test set of the WSIs for the best-performing graph (glomeruli + arteries) classification model configuration with each graph construction approach at the WSI level. The confusion matrices of all 5 test folds were aggregated and normalized.



(a) Hub-based

(b) Edge-weighted

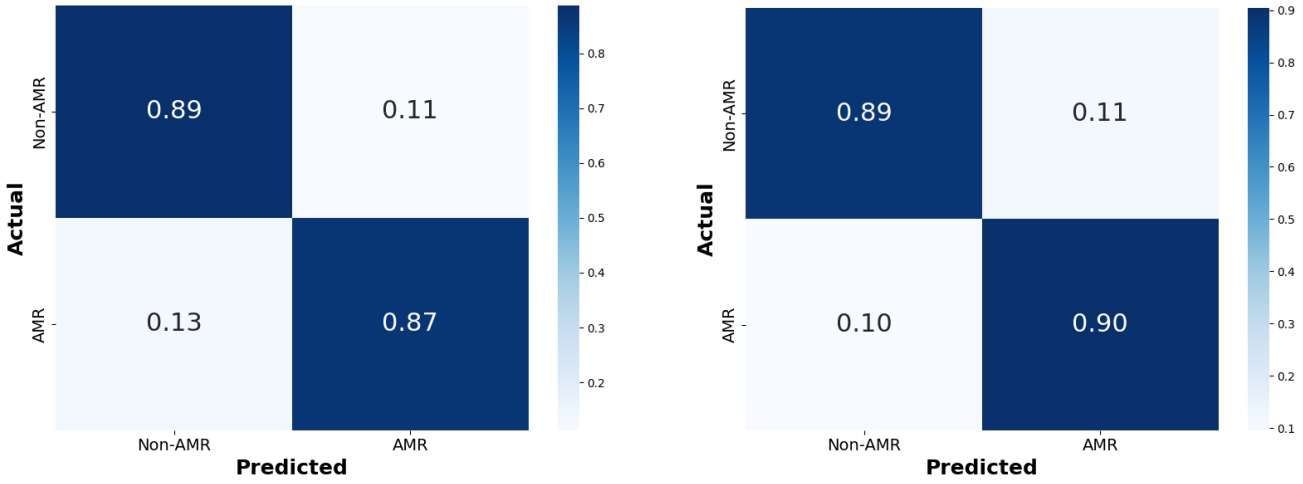
Fig. S.9. Normalized confusion matrix on the test set of the WSIs for the best-performing graph (glomeruli + arteries) classification model configuration with each graph construction approach at the biopsy level. The confusion matrices of all 5 test folds were aggregated and normalized.



(a) Hub-based

(b) Edge-weighted

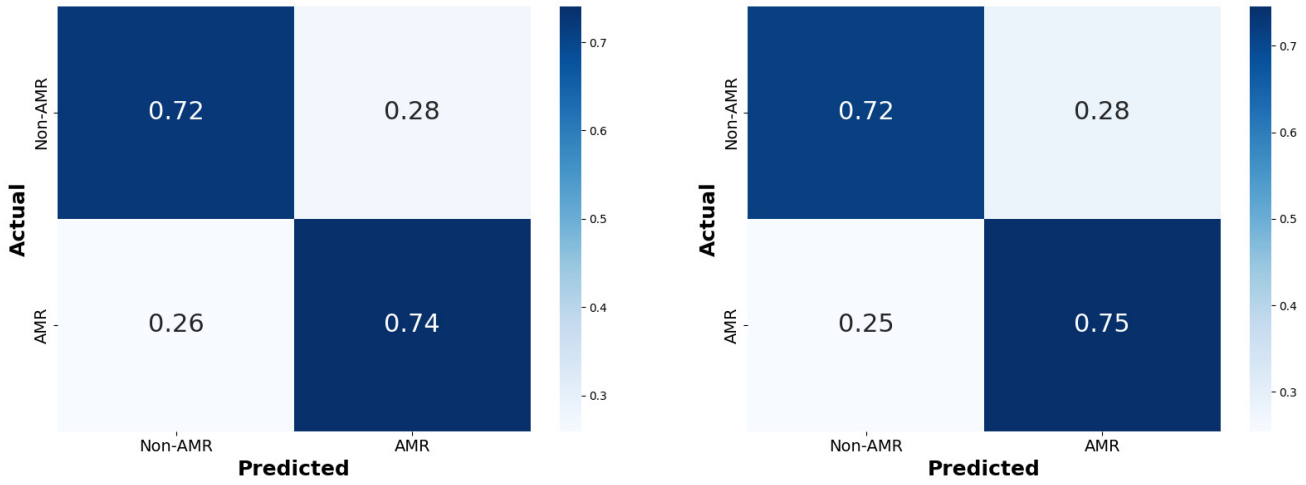
Fig. S.10. Normalized confusion matrix on the test set of the WSIs for the best-performing graph (glomeruli + cortical TI tiles) classification model configuration with each graph construction approach at the WSI level. The confusion matrices of all 5 test folds were aggregated and normalized.



(a) Hub-based

(b) Edge-weighted

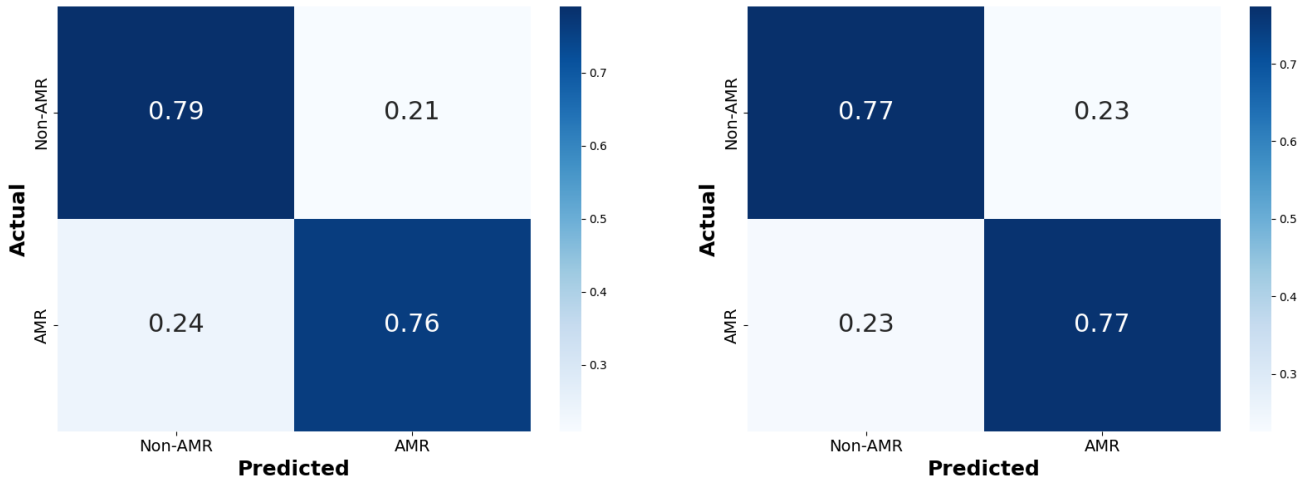
Fig. S.11. Normalized confusion matrix on the test set of the WSIs for the best-performing graph (glomeruli + cortical TI tiles) classification model configuration with each graph construction approach at the biopsy level. The confusion matrices of all 5 test folds were aggregated and normalized.



(a) Hub-based

(b) Edge-weighted

Fig. S.12. Normalized confusion matrix on the test set of the WSIs for the best-performing graph (glomeruli + arteries + cortical TI tiles) classification model configuration with each graph construction approach at the WSI level. The confusion matrices of all 5 test folds were aggregated and normalized.



(a) Hub-based

(b) Edge-weighted

Fig. S.13. Normalized confusion matrix on the test set of the WSIs for the best-performing graph (glomeruli + arteries + cortical TI tiles) classification model configuration with each graph construction approach at the biopsy level. The confusion matrices of all 5 test folds were aggregated and normalized.