

Supporting Information

Leakage-aware retrospective validation of a GWAS-informed drug repurposing pipeline for IgA nephropathy

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Supplementary Table 1. Protein-ligand co-folding confidence for the five top-ranked consensus candidates (three diffusion samples each).

Drug	Target	Model 0 ipTM	Model 1 ipTM	Model 2 ipTM	Mean ipTM	Contact Jaccard
Dasatinib	LYN	0.983	0.984	0.985	0.984	0.965
Bosutinib	LYN	0.984	0.983	0.980	0.982	0.893
Nintedanib	LYN	0.974	0.955	0.968	0.966	0.763
Masitinib	LYN	0.960	0.957	0.876	0.931	0.576
Tranilast	TGFB1	0.807	0.803	0.713	0.774	0.000

Predictions were generated with Boltz-2 (Passaro et al., 2025) using multiple-sequence-alignment context. ipTM is the ligand interface predicted TM-score. Contact Jaccard is the mean pairwise Jaccard similarity of contact residue sets across the three diffusion samples, with contacts defined as protein atoms within 4 angstroms of ligand heavy atoms. Source files: `results/boltz/confidence_summary.tsv` and `results/boltz/inter_model_rmsd.tsv` in the code and data archive (<https://doi.org/10.5281/zenodo.23098959>).