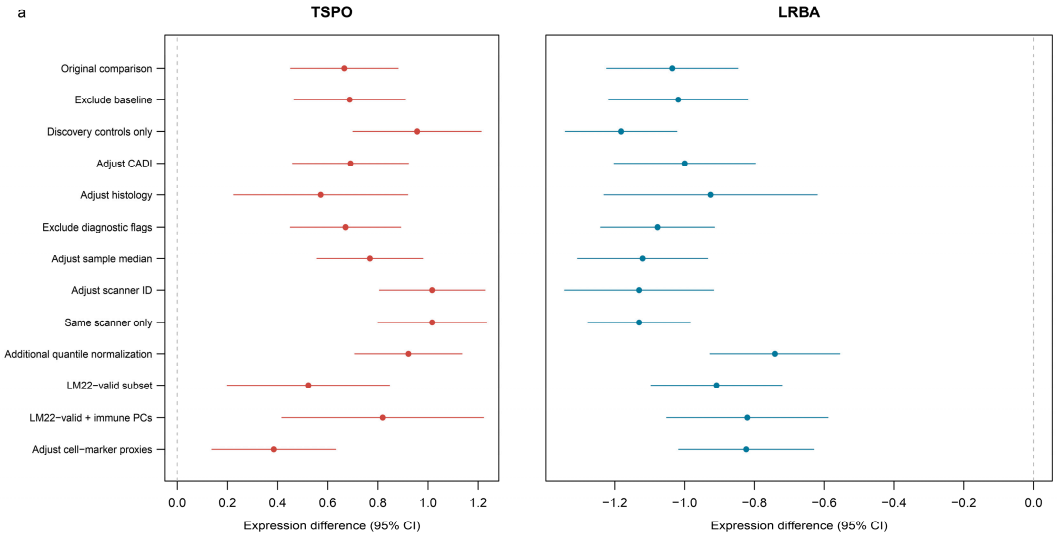
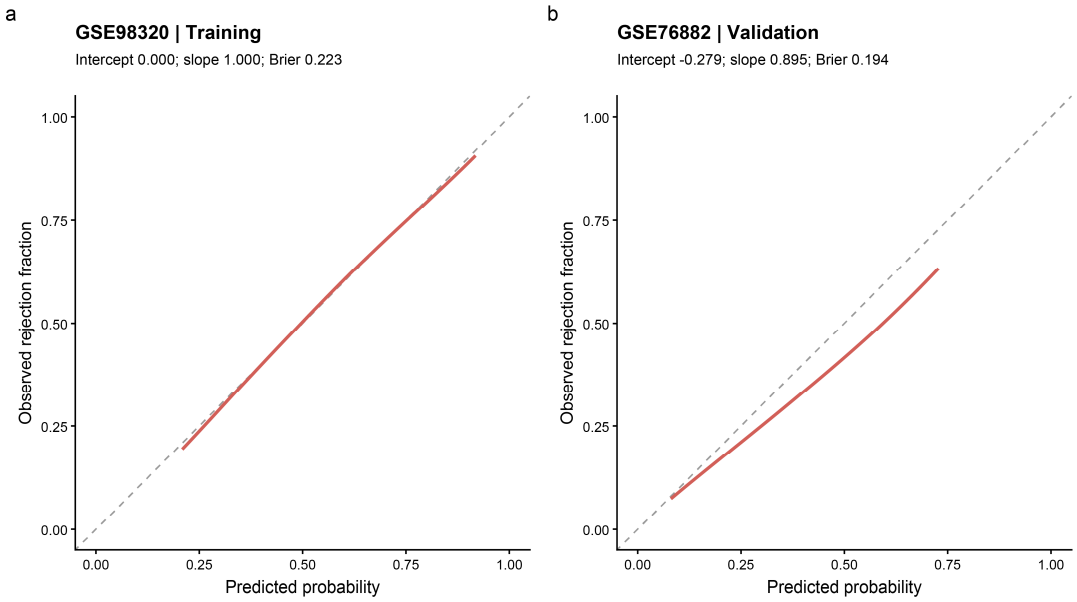
Figure S1



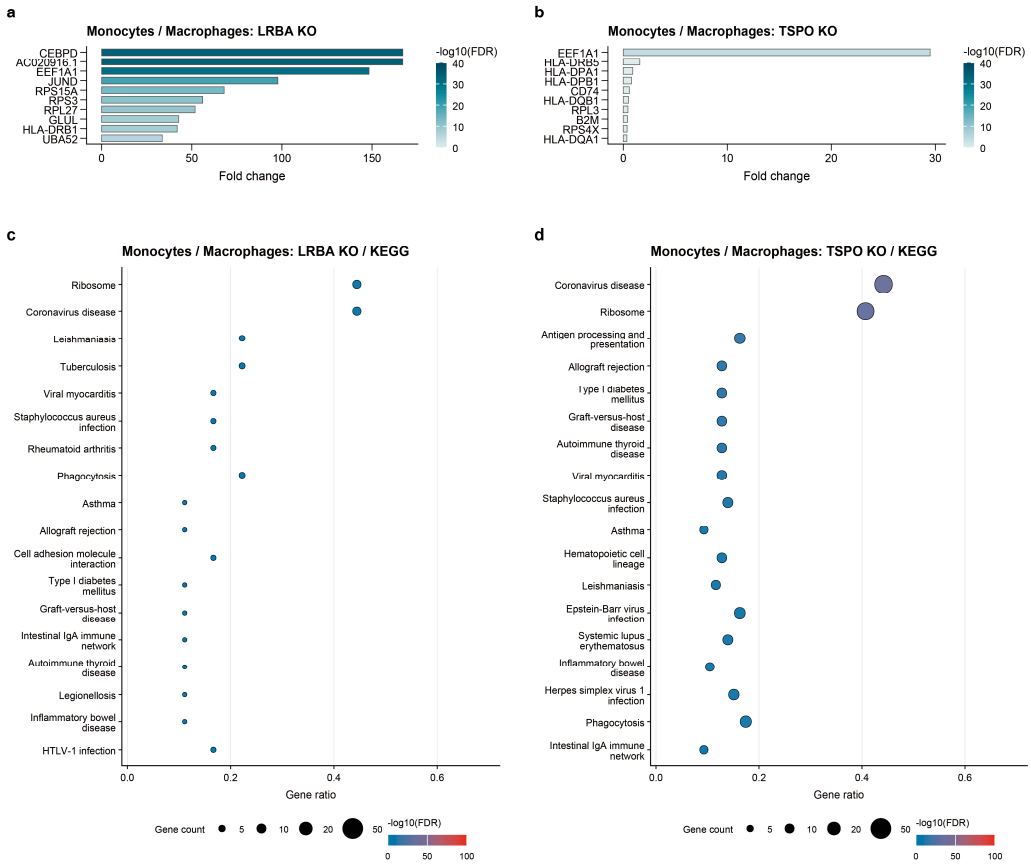
Supplementary Figure S1. Sensitivity analyses of TSPO and LRBA expression differences in GSE25902. Points show estimated log2 fold changes, and horizontal lines indicate 95% confidence intervals. Positive values indicate higher expression in rejection samples. Dashed lines indicate no difference.

Figure S2



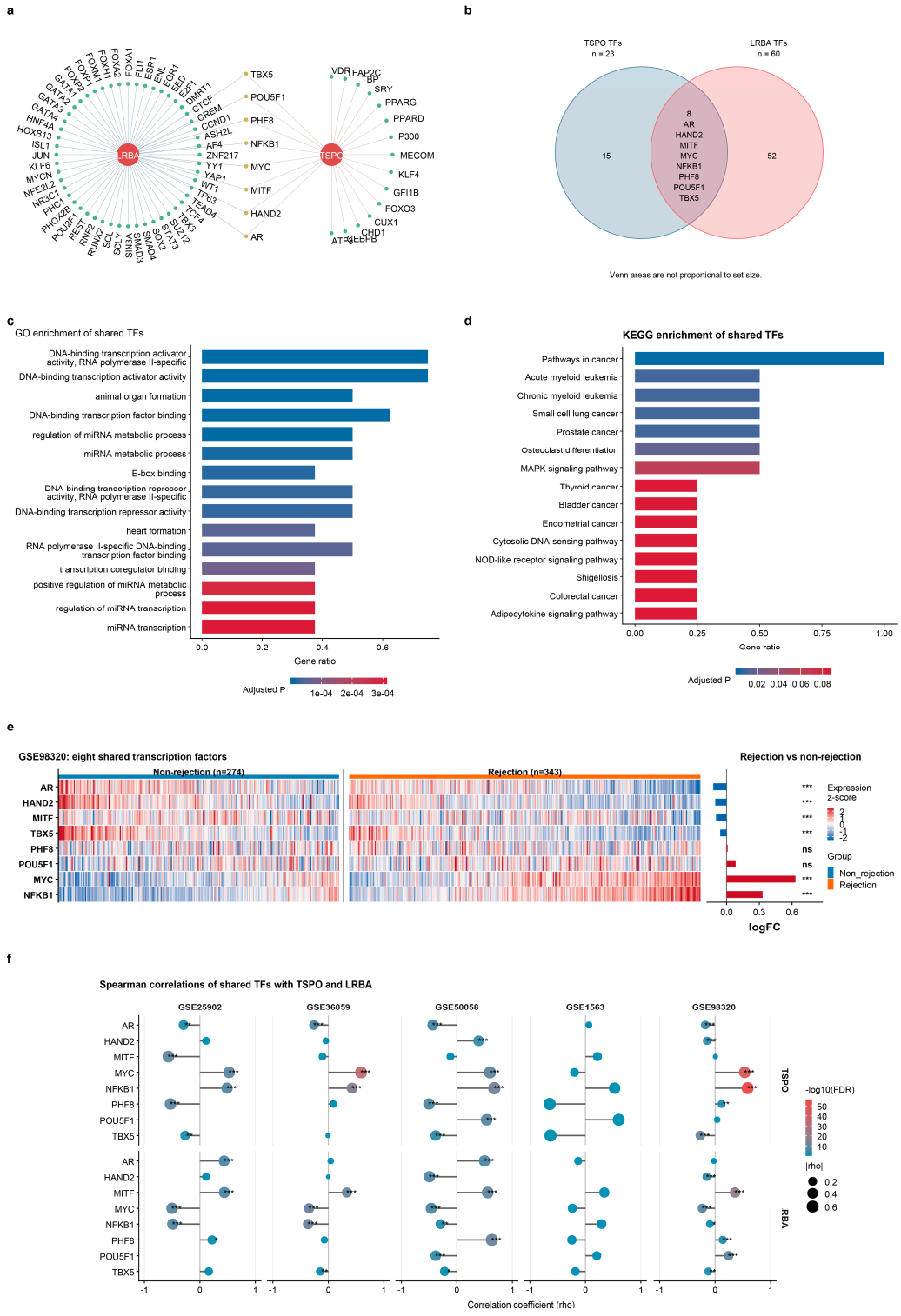
Supplementary Figures S2. **Calibration plots of the prediction model in the training and validation cohorts**. (a) GSE98320 training cohort . (b) GSE76882 validation cohort. The red lines show the relationship between predicted probabilities and observed rejection fractions. The dashed grey lines indicate perfect calibration. Calibration intercepts, slopes, and Brier scores are shown in each panel. The number of bootstrap resamples was 1,000.

Figure S3



Supplementary Figures S3. **Virtual knockout analysis of LRBA and TSPO in monocytes/macrophages using scTenifoldKnk.** (a,b) The ten most affected genes following scTenifoldKnk virtual knockout of LRBA and TSPO, respectively, in monocytes/macrophages. (c,d) KEGG enrichment results for genes affected by LRBA and TSPO virtual knockout, respectively, in monocytes/macrophages.

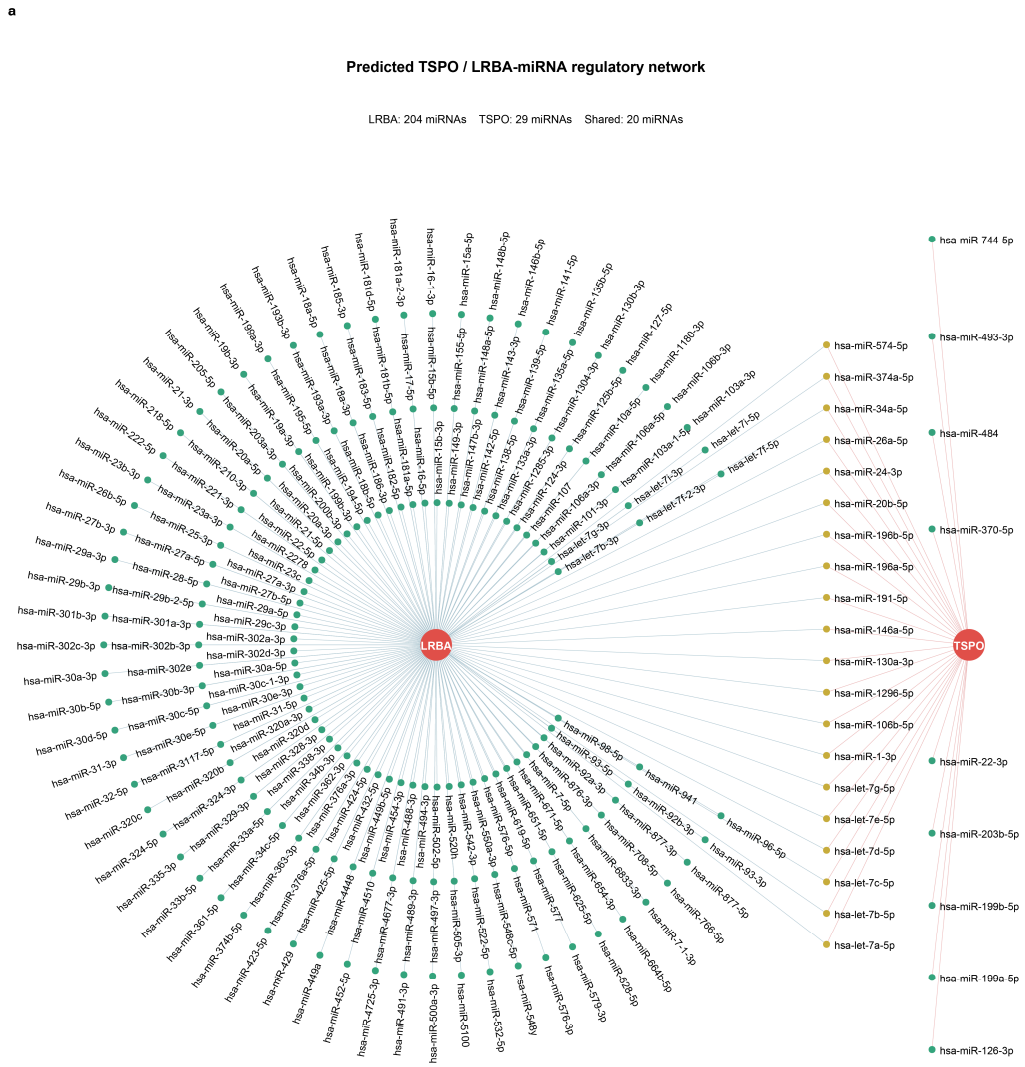
Figure S4



Supplementary Figures S4. Construction and functional analysis of the TSPO and LRBA transcription factor (TF) network. (a) Predicted links between transcription factors (TFs) and the target genes LRBA and TSPO. (b) Overlap of the TF lists for the

two genes, displayed in a Venn diagram. (c,d) Functional enrichment of the eight common TFs based on GO terms and KEGG pathways, respectively. (e) Heatmap of shared TF expression in GSE98320 rejection and non-rejection samples, together with differential expression summaries. (f) Associations of shared TF expression with TSPO and LRBA expression across cohorts. Expression differences were analysed with limma, and associations were evaluated by Spearman correlation. Within each cohort, P values underwent Benjamini–Hochberg correction.*adjusted $P < 0.05$; **adjusted $P < 0.01$; ***adjusted $P < 0.001$; ns, no significance.

Figure S5



Supplementary Figures S5. Construction of the hub gene-miRNA network. (a) Network showing microRNAs (miRNAs) that may target LRBA and TSPO. Red nodes represent the two target genes, green nodes represent miRNAs associated with one

target, and gold nodes represent miRNAs shared by both targets. Edges show predicted miRNA-target associations.

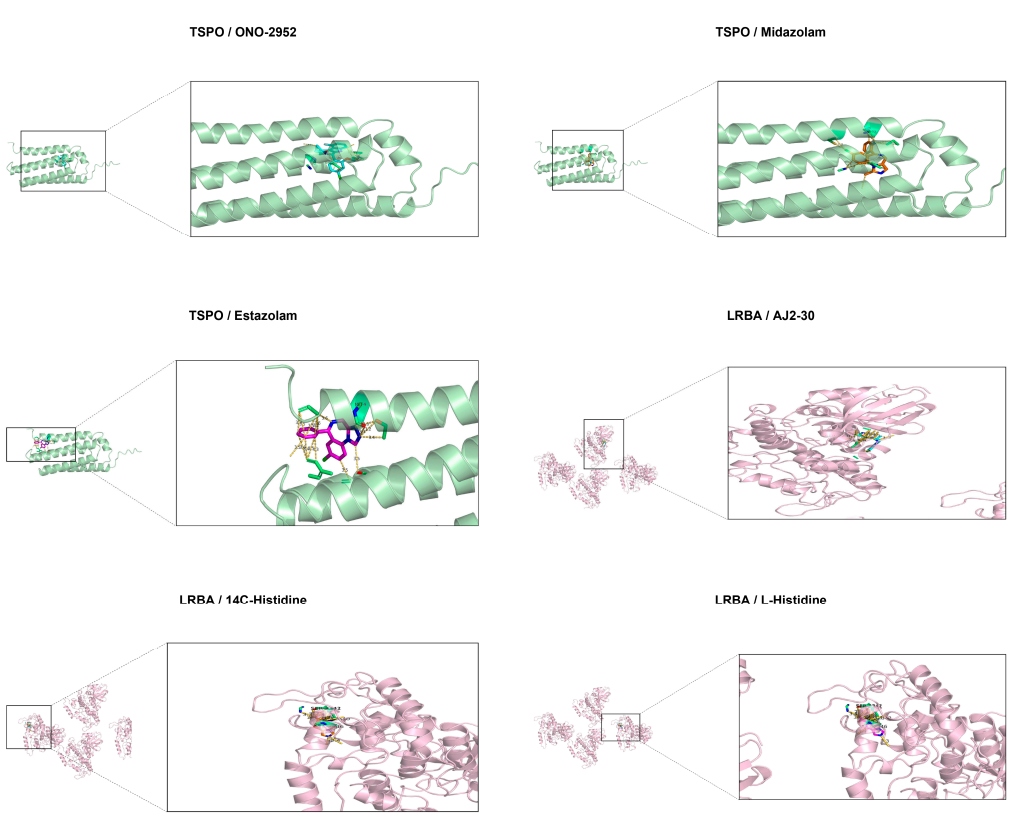
Figure S6

a

Gene	Gene source	Drug	PubChem CID	Vina score (kcal/mol)
LRBA	RCSB PDB 1T77	AJ2-30	163902400	-8.849
LRBA	RCSB PDB 1T77	14C-Histidine	-	-5.598
LRBA	RCSB PDB 1T77	L-Histidine	6274	-5.44
TSPO	AlphaFold AF-P30536-F1	ONO-2952	11524127	-8.581
TSPO	AlphaFold AF-P30536-F1	MIDAZOLAM	4192	-7.899
TSPO	AlphaFold AF-P30536-F1	ESTAZOLAM	3261	-7.283
TSPO	AlphaFold AF-P30536-F1	EMAPUNIL	6433109	-7.268
TSPO	AlphaFold AF-P30536-F1	FLUDIAZEPAM	3369	-7.155
TSPO	AlphaFold AF-P30536-F1	DIAZEPAM	3016	-7.086
TSPO	AlphaFold AF-P30536-F1	OXAZEPAM	4616	-7.019
TSPO	AlphaFold AF-P30536-F1	TRIAZOLAM	5556	-7.012
TSPO	AlphaFold AF-P30536-F1	LORAZEPAM	3958	-7.001
TSPO	AlphaFold AF-P30536-F1	FLUNITRAZEPAM	3380	-6.973
TSPO	AlphaFold AF-P30536-F1	HALAZEPAM	31640	-6.954

Gene	Gene source	Drug	PubChem CID	Vina score (kcal/mol)
TSPO	AlphaFold AF-P30536-F1	TEMAZEPAM	5391	-6.943
TSPO	AlphaFold AF-P30536-F1	CHLORDIAZEPOXIDE	2712	-6.862
TSPO	AlphaFold AF-P30536-F1	ESZOPICLONE	969472	-6.859
TSPO	AlphaFold AF-P30536-F1	CINOLAZEPAM	3033621	-6.83
TSPO	AlphaFold AF-P30536-F1	CLORAZEPIC ACID	2809	-6.664
TSPO	AlphaFold AF-P30536-F1	ALPRAZOLAM	2118	-6.66
TSPO	AlphaFold AF-P30536-F1	PRAZEPAM	4890	-6.535
TSPO	AlphaFold AF-P30536-F1	QUAZEPAM	4999	-6.521
TSPO	AlphaFold AF-P30536-F1	CLOTIAZEPAM	2811	-6.45
TSPO	AlphaFold AF-P30536-F1	ADINAZOLAM	37632	-6.326
TSPO	AlphaFold AF-P30536-F1	FLUMAZENIL	3373	-6.319
TSPO	AlphaFold AF-P30536-F1	ALPIDEM	54897	-5.893
TSPO	AlphaFold AF-P30536-F1	FLURAZEPAM	3393	-5.85
TSPO	AlphaFold AF-P30536-F1	CHLORMEZANONE	2717	-5.821

b



Supplementary Figures S6. Exploratory molecular docking of compounds associated with TSPO and LRBA. (a) Summary of candidate compounds, receptor structure sources, PubChem compound identifiers, and Vina docking scores. (b)

Representative docking poses showing TSPO with ONO-2952, midazolam, and estazolam, and LRBA with AJ2-30, 14C-histidine, and L-histidine.