Supplementary Notes for scEpiLock: A Weakly-Supervised Learning Framework for cis-Regulatory Element Localization and Variant Impact Quantification for Single-Cell Epigenetic Data

Yanwen Gong[1,2], Shushrruth Sai Srinivasan[3], Ruiyi Zhang[3], Kai Kessenbrock[1,2],* and Jing Zhang[3,*]

[1]Center for Complex Biological Systems, University of California, Irvine, CA 92697, USA
[2]Department of Biological Chemistry, School of Medicine, University of California, Irvine, CA 92697, USA
[3]Department of Computer Science, University of California, Irvine, CA 92697, USA

*To whom correspondence should be addressed.

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Note S1 Detailed specifications of the architectures and hyperparameters of scEpiLock multi-label classifier module

scEpiLock uses a multilayer CNN model, which contains four convolutional layers, two pooling layers and two dense fully connected layers. The filters in the convolutional layers are trained to recognize the CREs. The dense fully connected dense layers combine the learnt information and output the cell-type specific peak accessible score. The model is organized into a sequential layer-by-layer structure with each layer as a functional transformation.

Model Architecture:
1. Convolution layer (320 channels, kernel size 8, stride 1)
2. Convolution layer (480 channels, kernel size 8, stride 1)
3. Max pooling layer (kernel size 4, stride 4)
4. Convolution layer (960 channels, kernel size 4, stride 1)
5. Max pooling layer (kernel size 4, stride 4)
6. Convolution layer (1024 channels, kernel size 4, stride 1)
7. Fully connected layer1
8. Fully connected layer2

To avoid overfitting, we added dropouts to randomly set a proportion of neuron activations to a value of 0.

Dropout proportion (proportion of outputs randomly set to 0):
- Layer3: 20%
- Layer5: 50%
- Layer6: 50%
- Other layers: 0%

Supplementary Figures

Figure S1 Positive label distribution for each peak of PBMC
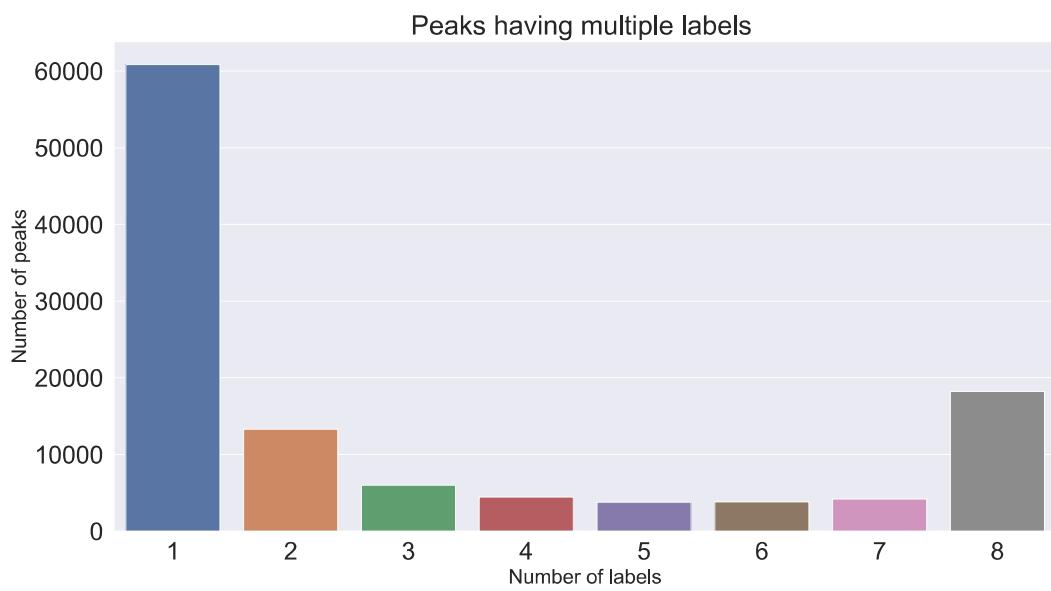
In the PBMC scATAC-seq data, 53.1% of peaks (n = 60,834 peaks) are unique to one cell type while 15.9% of peaks (n = 18,209 peaks) are shared among the eight cell types. Rest of the peaks are shared among two to seven cell types

Figure S2 Positive label distribution for each peak of the brain data

Peaks having multiple labels
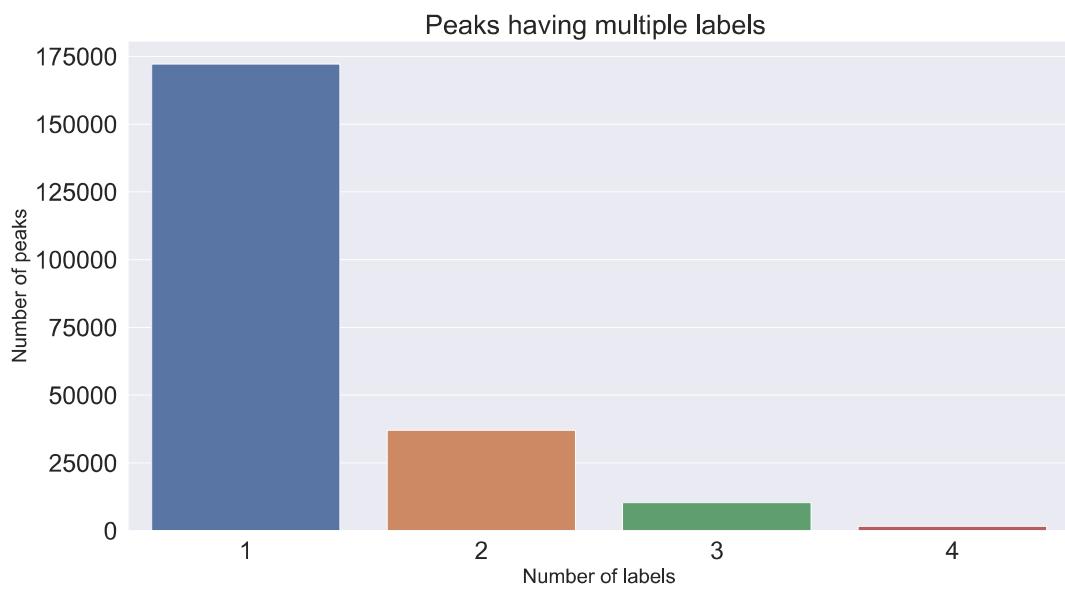
In the brain scATAC-seq data, 77.9% (n = 172,111 peaks) of peaks are specific to a single cell type and the rest of peaks are shared among at least two cell types

Supplementary Figure 3 Transfer learning improves multi-label classifier's performance on small scATAC-seq dataset
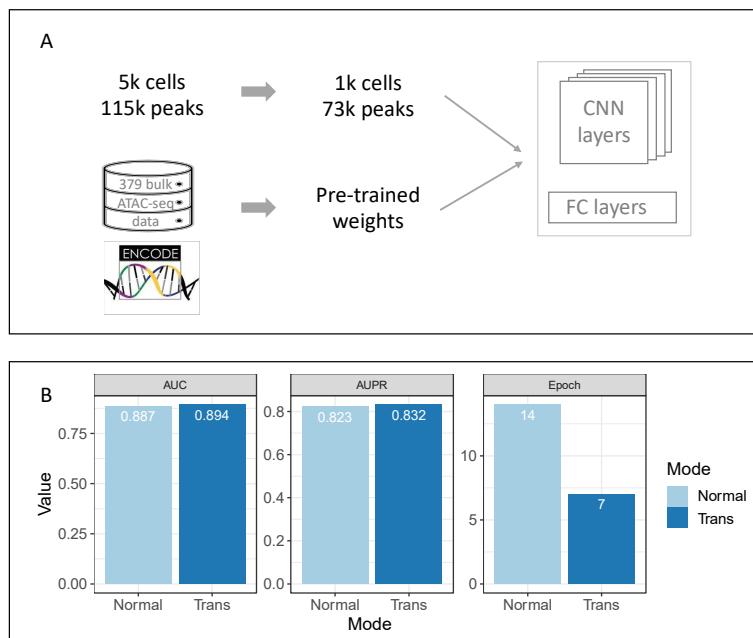
(A) ENCODE bulk ATAC-seq data was used to generate pre-trained weights of the classifier. The 5k PBMC data was filtered to only include 1k cells with 73k peaks representing a small scATAC-seq dataset. The pre-trained weights and subset dataset were fed into the multi-label classifier. (B) Transfer learning model achieved higher AUC and AUPR than model with random initiated weights. In addition, transfer learning reduced the training time to half of before.

Figure S4 Visualization of scEpiLock identified functional SNP rs10769263
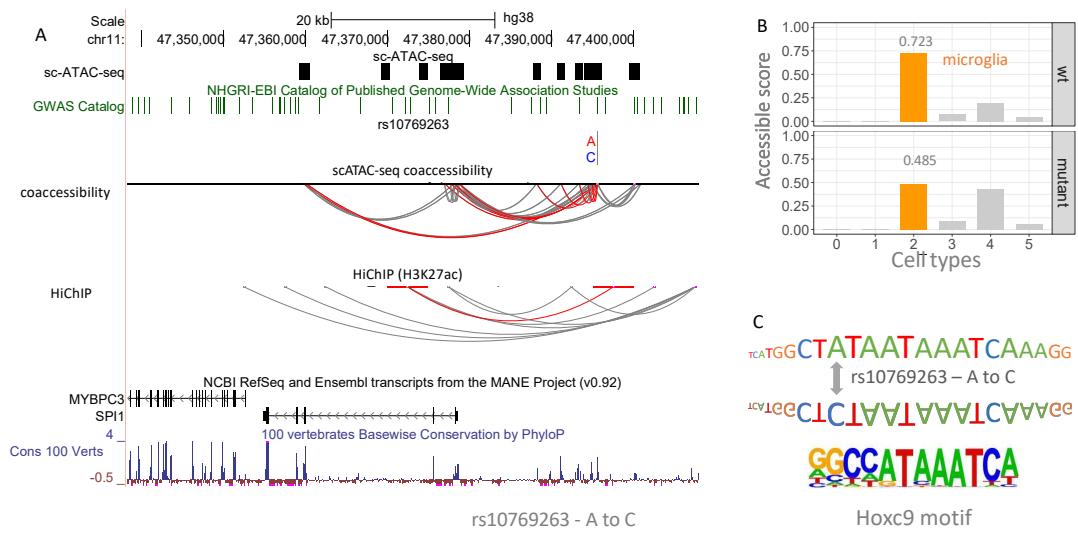
(A) Brain scATAC-seq pseudobulk, GWAS, rs10769263, co-accessibility, HiChIP, nearby genes, PhastCons 100 vertebrates track on UCSC genome browser. (B) Predicted accessible scores of WT and mutant. (C) Sequences contain rs10759263 SNP aligned with Hoxc9 motif logo

Table S1 ENCODE Bulk ATAC-seq Sample List for Transfer Learning

File.accession	Experiment.accession	File.download.URL
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ENCFF965AOW	ENCSR383RDZ	https://www.encodeproject.org/files/ENCFF965AOW/@@download/ENCFF965AOW.bed.gz
ENCFF007FSO	ENCSR684KUG	https://www.encodeproject.org/files/ENCFF007FSO/@@download/ENCFF007FSO.bed.gz
ENCFF132ATE	ENCSR368FYV	https://www.encodeproject.org/files/ENCFF132ATE/@@download/ENCFF132ATE.bed.gz
ENCFF110LOX	ENCSR220ASC	https://www.encodeproject.org/files/ENCFF110LOX/@@download/ENCFF110LOX.bed.gz
ENCFF008FUL	ENCSR220ASC	https://www.encodeproject.org/files/ENCFF008FUL/@@download/ENCFF008FUL.bed.gz
ENCFF181FFW	ENCSR220ASC	https://www.encodeproject.org/files/ENCFF181FFW/@@download/ENCFF181FFW.bed.gz
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ENCFF305ZQQ	ENCSR278JWM	https://www.encodeproject.org/files/ENCFF305ZQQ/@@download/ENCFF305ZQQ.bed.gz
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ENCFF182SEJ	ENCSR954BDA	https://www.encodeproject.org/files/ENCFF182SEJ/@@download/ENCFF182SEJ.bed.gz
ENCFF505YPT	ENCSR163KRG	https://www.encodeproject.org/files/ENCFF505YPT/@@download/ENCFF505YPT.bed.gz
ENCFF551EAY	ENCSR637MUF	https://www.encodeproject.org/files/ENCFF551EAY/@@download/ENCFF551EAY.bed.gz
ENCFF550WFX	ENCSR635AIF	https://www.encodeproject.org/files/ENCFF550WFX/@@download/ENCFF550WFX.bed.gz
ENCFF252MOE	ENCSR594TMY	https://www.encodeproject.org/files/ENCFF252MOE/@@download/ENCFF252MOE.bed.gz
ENCFF810XER	ENCSR040PBN	https://www.encodeproject.org/files/ENCFF810XER/@@download/ENCFF810XER.bed.gz
ENCFF471QJG	ENCSR833ACP	https://www.encodeproject.org/files/ENCFF471QJG/@@download/ENCFF471QJG.bed.gz
ENCFF246XGY	ENCSR000RBT	https://www.encodeproject.org/files/ENCFF246XGY/@@download/ENCFF246XGY.bed.gz
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ENCFF695IGF	ENCSR483RKN	https://www.encodeproject.org/files/ENCFF695IGF/@@download/ENCFF695IGF.bed.gz
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ENCFF522FNJ	ENCSR373TDL	https://www.encodeproject.org/files/ENCFF522FNJ/@@download/ENCFF522FNJ.bed.gz
ENCFF199VHV	ENCSR563ZNI	https://www.encodeproject.org/files/ENCFF199VHV/@@download/ENCFF199VHV.bed.gz
ENCFF455PLR	ENCSR788TRR	https://www.encodeproject.org/files/ENCFF455PLR/@@download/ENCFF455PLR.bed.gz
ENCFF963YOX	ENCSR788TRR	https://www.encodeproject.org/files/ENCFF963YOX/@@download/ENCFF963YOX.bed.gz
ENCFF431CPR	ENCSR072UYN	https://www.encodeproject.org/files/ENCFF431CPR/@@download/ENCFF431CPR.bed.gz
ENCFF277OGS	ENCSR072UYN	https://www.encodeproject.org/files/ENCFF277OGS/@@download/ENCFF277OGS.bed.gz
ENCFF203EQG	ENCSR152PSA	https://www.encodeproject.org/files/ENCFF203EQG/@@download/ENCFF203EQG.bed.gz
ENCFF804EIN	ENCSR152PSA	https://www.encodeproject.org/files/ENCFF804EIN/@@download/ENCFF804EIN.bed.gz
ENCFF873GXL	ENCSR210NKB	https://www.encodeproject.org/files/ENCFF873GXL/@@download/ENCFF873GXL.bed.gz
ENCFF643ZJJ	ENCSR210NKB	https://www.encodeproject.org/files/ENCFF643ZJJ/@@download/ENCFF643ZJJ.bed.gz
ENCFF305GIG	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF305GIG/@@download/ENCFF305GIG.bed.gz
ENCFF760HHY	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF760HHY/@@download/ENCFF760HHY.bed.gz
ENCFF545AQB	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF545AQB/@@download/ENCFF545AQB.bed.gz
ENCFF222VTK	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF222VTK/@@download/ENCFF222VTK.bed.gz
ENCFF530FMG	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF530FMG/@@download/ENCFF530FMG.bed.gz
ENCFF748OSQ	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF748OSQ/@@download/ENCFF748OSQ.bed.gz
ENCFF966AKO	ENCSR868FGK	https://www.encodeproject.org/files/ENCFF966AKO/@@download/ENCFF966AKO.bed.gz
ENCFF912MCC	ENCSR516CPW	https://www.encodeproject.org/files/ENCFF912MCC/@@download/ENCFF912MCC.bed.gz
ENCFF300UPI	ENCSR846VPV	https://www.encodeproject.org/files/ENCFF300UPI/@@download/ENCFF300UPI.bed.gz

ENCFF303AKJ	ENCSR846VPV	https://www.encodeproject.org/files/ENCFF303AKJ/@@download/ENCFF303AKJ.bed.gz
ENCFF882FLC	ENCSR422SUG	https://www.encodeproject.org/files/ENCFF882FLC/@@download/ENCFF882FLC.bed.gz
ENCFF204NII	ENCSR422SUG	https://www.encodeproject.org/files/ENCFF204NII/@@download/ENCFF204NII.bed.gz
ENCFF882OVP	ENCSR422SUG	https://www.encodeproject.org/files/ENCFF882OVP/@@download/ENCFF882OVP.bed.gz
ENCFF905GGG	ENCSR422SUG	https://www.encodeproject.org/files/ENCFF905GGG/@@download/ENCFF905GGG.bed.gz
ENCFF885TNX	ENCSR308HPZ	https://www.encodeproject.org/files/ENCFF885TNX/@@download/ENCFF885TNX.bed.gz
ENCFF461RJQ	ENCSR308HPZ	https://www.encodeproject.org/files/ENCFF461RJQ/@@download/ENCFF461RJQ.bed.gz
ENCFF791RKW	ENCSR042AWH	https://www.encodeproject.org/files/ENCFF791RKW/@@download/ENCFF791RKW.bed.gz
ENCFF851SSE	ENCSR042AWH	https://www.encodeproject.org/files/ENCFF851SSE/@@download/ENCFF851SSE.bed.gz
ENCFF314RIW	ENCSR042AWH	https://www.encodeproject.org/files/ENCFF314RIW/@@download/ENCFF314RIW.bed.gz
ENCFF438JMM	ENCSR042AWH	https://www.encodeproject.org/files/ENCFF438JMM/@@download/ENCFF438JMM.bed.gz
ENCFF133HUE	ENCSR040DJK	https://www.encodeproject.org/files/ENCFF133HUE/@@download/ENCFF133HUE.bed.gz
ENCFF784MGH	ENCSR040DJK	https://www.encodeproject.org/files/ENCFF784MGH/@@download/ENCFF784MGH.bed.gz
ENCFF278WQH	ENCSR201FIW	https://www.encodeproject.org/files/ENCFF278WQH/@@download/ENCFF278WQH.bed.gz
ENCFF675XYC	ENCSR201FIW	https://www.encodeproject.org/files/ENCFF675XYC/@@download/ENCFF675XYC.bed.gz
ENCFF356UPB	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF356UPB/@@download/ENCFF356UPB.bed.gz
ENCFF774JIK	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF774JIK/@@download/ENCFF774JIK.bed.gz
ENCFF193HEJ	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF193HEJ/@@download/ENCFF193HEJ.bed.gz
ENCFF164FNM	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF164FNM/@@download/ENCFF164FNM.bed.gz
ENCFF049BCQ	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF049BCQ/@@download/ENCFF049BCQ.bed.gz
ENCFF385QXA	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF385QXA/@@download/ENCFF385QXA.bed.gz
ENCFF368MPK	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF368MPK/@@download/ENCFF368MPK.bed.gz
ENCFF169RTS	ENCSR551CSY	https://www.encodeproject.org/files/ENCFF169RTS/@@download/ENCFF169RTS.bed.gz
ENCFF912IDR	ENCSR607BTF	https://www.encodeproject.org/files/ENCFF912IDR/@@download/ENCFF912IDR.bed.gz
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ENCFF461IGU	ENCSR241OBO	https://www.encodeproject.org/files/ENCFF461IGU/@@download/ENCFF461IGU.bed.gz
ENCFF315XZD	ENCSR241OBO	https://www.encodeproject.org/files/ENCFF315XZD/@@download/ENCFF315XZD.bed.gz
ENCFF679YNL	ENCSR404LLJ	https://www.encodeproject.org/files/ENCFF679YNL/@@download/ENCFF679YNL.bed.gz
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ENCFF913BUA	ENCSR831KAH	https://www.encodeproject.org/files/ENCFF913BUA/@@download/ENCFF913BUA.bed.gz
ENCFF623GOH	ENCSR831KAH	https://www.encodeproject.org/files/ENCFF623GOH/@@download/ENCFF623GOH.bed.gz

ENCFF510PGR	ENCSR761TKU	https://www.encodeproject.org/files/ENCFF510PGR/@@download/ENCFF510PGR.bed.gz
ENCFF668ARP	ENCSR761TKU	https://www.encodeproject.org/files/ENCFF668ARP/@@download/ENCFF668ARP.bed.gz
ENCFF235JZB	ENCSR200OML	https://www.encodeproject.org/files/ENCFF235JZB/@@download/ENCFF235JZB.bed.gz
ENCFF383XOM	ENCSR200OML	https://www.encodeproject.org/files/ENCFF383XOM/@@download/ENCFF383XOM.bed.gz
ENCFF114GDS	ENCSR200OML	https://www.encodeproject.org/files/ENCFF114GDS/@@download/ENCFF114GDS.bed.gz
ENCFF982UNH	ENCSR200OML	https://www.encodeproject.org/files/ENCFF982UNH/@@download/ENCFF982UNH.bed.gz
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ENCFF250ANB	ENCSR996ZCR	https://www.encodeproject.org/files/ENCFF250ANB/@@download/ENCFF250ANB.bed.gz
ENCFF775HDQ	ENCSR153IUB	https://www.encodeproject.org/files/ENCFF775HDQ/@@download/ENCFF775HDQ.bed.gz
ENCFF173AVZ	ENCSR153IUB	https://www.encodeproject.org/files/ENCFF173AVZ/@@download/ENCFF173AVZ.bed.gz
ENCFF816GCG	ENCSR670REK	https://www.encodeproject.org/files/ENCFF816GCG/@@download/ENCFF816GCG.bed.gz
ENCFF456JOB	ENCSR670REK	https://www.encodeproject.org/files/ENCFF456JOB/@@download/ENCFF456JOB.bed.gz
ENCFF822SDP	ENCSR851SBY	https://www.encodeproject.org/files/ENCFF822SDP/@@download/ENCFF822SDP.bed.gz
ENCFF430VEQ	ENCSR851SBY	https://www.encodeproject.org/files/ENCFF430VEQ/@@download/ENCFF430VEQ.bed.gz

Table S2 Computing Power and Processing Time for Each Model

Computation power	Model	PBMC	Brain
One GPU	**scEpiLock**	1:39:53	4:14:56
	DeepSEA	1:06:06	2:47:59
	DanQ	1:19:02	3:23:34
One CPU	Random forest	0:06:25	0:07:54

Table S3 H3K27ac Enrichment in Key and Non-key Regions

Data	Region	H3K27ac enrichment	p-value
PBMC	key	0.554	<2.2e-16
	Non-key	0.412	
Brain	key	1.448	<2.2e-16
	Non-key	0.987	