

Supplementary Materials for

Computational methods for the prediction of chromatin interaction and organization using sequence and epigenomic profiles

Huan Tao ^{1,†}, Hao Li ^{1,†}, Kang Xu ¹, Hao Hong ¹, Shuai Jiang ¹, Guifang Du ¹, Junting Wang ¹, Yu Sun ¹, Xin Huang ¹, Yang Ding ¹, Fei Li ², Xiaofei Zheng ^{1,*}, Hebing Chen ^{1,*} and Xiaochen Bo ^{1,*}

1 Beijing Institute of Radiation Medicine, Beijing 100850, China.

2 Computer Network Information Center, Chinese Academy of Sciences, Beijing 100190, China.

* To whom correspondence should be addressed. Tel: +8601066932251; Email: boxc@bmi.ac.cn (X.B.).

Correspondence may also be addressed to chb-1012@163.com (H.C.) and xfzheng100@126.com (X.Z.).

†The authors wish it to be known that, in their opinion, the first two authors should be regarded as Joint First Authors.

The PDF file includes:

Table S1. Code availability of computational methods for the prediction of chromatin interaction and organization.

Table S2. Required input data of computational methods for the prediction of chromatin interaction and organization.

Table S3. Databases of available predictions supplied by computational methods.

Table S1 Code availability of computational methods for the prediction of chromatin interaction and organization

| Tool Name | URLs | Implementation |
|--|--|----------------|
| Computational methods for the prediction of chromatin interaction | | |
| Unsupervised Methods | | |
| PreSTIGE | http://prestige.case.edu | Web software |
| ABC | https://github.com/broadinstitute/ABC-Enhancer-Gene-Prediction | Python |
| Ernst et al. | / | / |
| Thurman et al. | / | / |
| ELMER | https://github.com/lijingya/ELMER http://bioconductor.org/packages/ELMER | R |
| Naville et al. | https://github.com/DyogenIBENS/Regulus | Python |
| CISMAPPER | / | / |
| Cicero | https://github.com/cole-trapnell-lab/cicero-release | R |
| C3D | https://github.com/LupienLab/C3D | BASH and R |
| EpiTensor | / | MACS2 |
| CITD | https://cb.utdallas.edu/CITD/index.htm | / |
| SWIPE-NMF | https://github.com/kaiyuanmifen/SWIPE-NMF | R |
| Supervised Methods | | |
| JEME | https://github.com/yiplabcuhk/JEME/ | R, Weka |
| FOCS | https://github.com/Shamir-Lab/FOCS | R |
| IM-PET | www.healthcare.uiowa.edu/labs/tan/IM-PET_Package.tgz | / |
| RIPPLE | http://pages.discovery.wisc.edu/~sroy/ripple/download.html | C++, Matlab |
| PETModule | http://hulab.ucf.edu/research/projects/PETModule/ | Python |
| TargetFinder | https://github.com/shwhalen/targetfinder | Python |
| McEnhancer | https://ohlerlab.mdc-berlin.de/software/McEnhancer_134/ | Python |
| CISD | https://github.com/huizhangucas/CISD | BASH, R |
| EP_Bayes | https://github.com/ManchesterBioinference/EP_Bayes | Python, R |

| | | |
|-----------------|--|-----------------|
| 3DEpiLoop | https://bitbucket.org/4dnucleome/3depiloop | R |
| Multi-levels 3D | / | / |
| CRUP | https://github.com/VerenaHeinrich/CRUP https://zenodo.org/record/3469676#.XzOQyDMpWmQ | R |
| EAGLE | https://github.com/EvansGao/EAGLE | Perl, Matlab |
| DeepTACT | / | / |
| EPIP | http://www.cs.ucf.edu/~xiaoman/EPIP/ | Python |
| 3DPredictor | https://github.com/labdevgen/3Dpredictor | Python, R, Java |
| PEP | http://acgt.cs.tau.ac.il/focs | Python |
| EPIANN | https://github.com/wgmao/EPIANN | Python, R |
| EP2vec | https://github.com/wanwenzeng/ep2vec | Python |
| SPEID | https://github.com/macompbio/ | Python |
| EnContact | https://github.com/liwenran/EnContact | Python |

Computational methods for the prediction of chromatin organization

Loops

| | | |
|-----------|---|------------|
| CISD-loop | https://github.com/huizhangucas/CISD | BASH and R |
| CTCF-MP | https://github.com/ma-compbio/CTCF-MP | Python |
| Lollipop | https://github.com/ykai16/Lollipop | Python |
| DeepMILO | https://github.com/khuranalab/DeepMILO | Python |

TADs

| | | |
|-------------|---|--------|
| CITD | https://cb.utdallas.edu/CITD/index.htm | / |
| PGSA | / | / |
| TAD-Lactuca | https://github.com/LoopGan/TAD-Lactuca | Python |
| nTDP | http://www.cs.cmu.edu/~ckingsf/research/ntdp | Python |
| BART | https://github.com/huangjialiangan/HubPredictor | R |

Contact map

| | | |
|----------|---|---|
| Rambutan | / | / |
|----------|---|---|

| | | |
|--------------|--|--------------------------------|
| Farré et al. | Keras package (https://github.com/keras-team/keras) TensorFlow (https://www.tensorflow.org/). | Python |
| Akita | https://github.com/calico/basenji/tree/master/manuscripts/akita | Python |
| DeepC | https://github.com/rschwess/deepC | Python, tensorflow, R and Perl |

3D structures

| | | |
|------------------------------|---|--|
| MiChroM | / | / |
| HiP-HoP | https://www.sciencedirect.com/science/article/pii/S1097276518307871?via%3Dihub#sec4.1c | LAMMPS, Bowtie2, SAMtools, BEDtools, MACS2. etc. |
| Chromatin states-based model | https://github.com/ZhangGroup-MITChemistry/DRAGON | LAMMPS |
| Bkhetan et al. | / | / |

Table S2 Required input data of computational methods for the prediction of chromatin interaction and organization

| | DNA sequence | DNA methylation | Distance | CTCF | Cohesin | p300 | RNAP II | TF binding | Chromatin Accessibility | | | | Histone Marks | | | | TAD | HiC | Gene Expression |
|--|--------------|-----------------|----------|------|---------|------|---------|------------|-------------------------|----------|-----------|-----------|---------------|----------|---------|----------|-----|----------|-----------------|
| | | | | | | | | | DHS | ATAC-seq | MNase-seq | FAIRE-seq | H3K4me1 | H3K4me3 | H3K27ac | Other | | | |
| Computational methods for the prediction of chromatin interaction | | | | | | | | | | | | | | | | | | | |
| PreSTIGE | | | √ | √ | | | | | | | | | √ | | | | | √ | |
| ABC | | | √ | √ | | | | | √ | <i>N</i> | | | | | √ | | | <i>/</i> | |
| Ernst et al. | | | √ | √ | | | √ | √ | | | | | √ | √ | √ | √ | | √ | |
| Thurman et al. | | √ | √ | | | | | √ | √ | | | | | √ | | | | √ | |
| ELMER | | √ | | | | | | | | | | | | | | | | √ | |
| Naville et al. | | | √ | | | √ | | √ | √ | | | | √ | √ | √ | | | | |
| CISMAPPER | | | <i>/</i> | | | | | √ | | | | | | <i>/</i> | √ | <i>/</i> | | √ | |
| Cicero | | | √ | | | | | | | √ | | | | | | | | | |
| C3D | | | | | | | | | √ | | | | | | | | | | |
| EpiTensor | | | | | | | | | √ | | | | √ | √ | √ | √ | √ | √ | |
| CITD | | | | √ | | | | √ | | | | | √ | √ | √ | √ | | √ | |
| SWIPE-NMF | | | | √ | | | | √ | √ | | | | √ | √ | √ | √ | √ | √ | |
| JEME | | √ | √ | | | | | | √ | | | | √ | √ | √ | | | √ | |
| FOCS | | √ | √ | | | | | | √ | | | | | | | | | √ | |
| IM-PET | √ | | √ | | | √ | | √ | <i>/</i> | | | | √ | √ | √ | | | √ | |
| RIPPLE | | | | | | | | √ | √ | | | | √ | √ | √ | √ | | √ | |
| PETModule | | | √ | | | √ | | √ | √ | | | | | | | | | | |
| TargetFinder | | √ | | √ | √ | √ | | √ | √ | | | √ | √ | √ | √ | √ | | √ | |

| | | | | | | | | | | | | | | | | | | | |
|----------------------------------|---|--|--|---|---|--|---|---|---|---|--|--|---|---|---|---|--|--|--|
| TAD–Lactuca | √ | | | √ | | | | | | | | | √ | √ | √ | √ | | | |
| nTDP | | | | | | | | | / | | | | √ | √ | / | √ | | | |
| BART | / | | | √ | | | | | | | | | √ | √ | √ | √ | | | |
| Rambutan | √ | | | | | | | | √ | | | | | | | | | | |
| Farré et al. | √ | | | √ | | | √ | √ | | | | | √ | √ | √ | √ | | | |
| Akita | √ | | | | | | | | | | | | | | | | | | |
| DeepC | √ | | | | | | | | | | | | | | | | | | |
| MiChroM | | | | | | | | | | | | | √ | √ | √ | √ | | | |
| HiP-HoP | | | | √ | / | | | | | √ | | | | | √ | | | | |
| Chromatin states- Based model | | | | √ | / | | | | √ | | | | √ | √ | √ | √ | | | |
| Bkhetan et al. | √ | | | √ | √ | | / | √ | | | | | √ | √ | | √ | | | |

(/ presents optional, /√ presents or)

Table S3 Databases of available predictions supplied by computational methods

| Number | Tool Name | Brief Description | URLs |
|---------------|------------------|---|---|
| 1 | PreSTIGE | Predicted enhancer-gene pairs for 13 cell lines | https://genetics.cwru.edu/prestige/ |
| 2 | JEME | Enhancer-promoter network in 935 samples of human primary cells, tissues and cell lines | http://yiplab.cse.cuhk.edu.hk/jeme/ |
| 3 | FOCS | Extensive enhancer-promotor maps of 2630 samples taken from ENCODE, Roadmap Epigenomics, FANTOM5, and a new compendium of GRO-seq | http://acgt.cs.tau.ac.il/focs/ |
| 4 | EnContact | 1,545,180 positive EEI predicted in seven cell lines | https://github.com/liwenran/EnContact |
| 5 | EAGLE | 7,680,203 enhancer-gene interactions involving 31,375 genes and 138,547 enhancers across 89 tissue/cell types in mouse; 7,437,255 enhancer-gene interactions involving 43,724 genes and 177,062 enhancers across 110 tissue/cell types in human | https://enhanceratlas.org/ |
| 6 | CITD | Chromatin interaction, topological domains and their states on 100 cell types from ENCODE and Roadmap with different resolutions | https://cb.utdallas.edu/CITD/index.htm |
| 7 | PETModule | Predicted ETGs in 8 human cells and 2 mouse cells | http://hulab.ucf.edu/research/projects/PETModule/ |
| 8 | SWIPE-NMF | Enhancer-promoter network in 127 human cell lines | https://dataverse.harvard.edu/dataset.xhtml?persistentId=doi:10.7910/DVN/DNBBB2 |
