Processed human microRNA-overexpression data from GEO, and sequence information from TargetScan, and targetScore from TargetScore

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1 MicroRNA perturbation datasets

\$`GEO Series`

We collected 84 Gene Expression Omnibus (GEO) series corresponding to 6 platforms, 77 human cells or tissues, and 112 distinct miRNAs. To our knowledge, this is by far the largest miRNA-overexpression data compendium. To automate the data download and processing, we developed a pipeline written in R, making use of the function getGEO from *GEOquery* R/Bioconductor package (Davis and Meltzer [2007]). For each dataset, the pipeline downloads the raw or processed data (if available) and calculates (when necessary) the log fold-change (logFC) in treatment (miRNA transfected) vs (mock) control, taking into account the unique properties of each data. Next, we combined all of the logFC data columns into a single $N \times M$ matrix for all of the N=19177 RefSeq mRNAs (NM_* obtained from UCSC) and M=286 datasets. Missing data (logFC) for some genes across studies were imputed using impute.knn from *impute* R package (Troyanskaya et al. [2001]). For miRNA transfection data having multiple measurements (in different studies), we picked the one whose logFC correlate the most with the validated targets from mirTarBase Hsu et al. [2011] or average them if no validated target available.

```
[1] 84

$Platform

[1] 6

$`Cell/Tissue`

[1] 77
```

2 TargetScan context score and PCT

TargetScan context score and PCT for all of the predicted sites (including conserved and nonconserved sites) downloaded from TargetScan website (http://www.targetscan.org/cgi-bin/targetscan/data_download.cgi?db=vert_61)

```
> targetScanCS <- get_TargetScanHuman_contextScore()
```

- > targetScanPCT <- get_TargetScanHuman_PCT()</pre>
- > head(targetScanCS)

```
Gene Symbol Transcript ID
                                       miRNA 3prime pairing local AU position
1
         A1CF
                  NM_138932 hsa-miR-4711-3p
                                                      -0.018
                                                               -0.095
                                                                         -0.10
2
         A1CF
                  NM_138933 hsa-miR-4711-3p
                                                               -0.095
                                                                         -0.10
                                                      -0.018
3
         A1CF
                  NM_014576 hsa-miR-4711-3p
                                                      -0.018
                                                               -0.095
                                                                         -0.10
4
                                                                         -0.10
         A1CF
               NM_001198820 hsa-miR-4711-3p
                                                      -0.018
                                                               -0.095
5
               NM_001198819 hsa-miR-4711-3p
                                                                         -0.10
         A1CF
                                                      -0.018
                                                                -0.095
6
         A1CF
               NM_001198818 hsa-miR-4711-3p
                                                                -0.095
                                                                         -0.10
                                                      -0.018
          SPS context+ score context+ score percentile
     TΑ
1 0.003 0.017
                       -0.448
                                                      99
2 0.003 0.017
                      -0.448
                                                      99
                                                      99
3 0.003 0.017
                      -0.448
```

99

99

99

> dim(targetScanCS)

4 0.003 0.017

5 0.003 0.017

6 0.003 0.017

[1] 9569357 10

> head(targetScanPCT)

```
miR Family Gene Symbol Transcript ID
                                                   PCT
1
         miR-22/22-3p
                              A1BG
                                       NM_130786 0.00
2
     miR-23abc/23b-3p
                                       NM_130786 0.00
                              A1BG
7
  miR-26ab/1297/4465
                              A1BG
                                       NM_130786 0.00
8
        miR-101/101ab
                                       NM_130786 0.00
                              A1BG
  miR-103a/107/107ab
                              A1BG
                                       NM_130786 0.00
10 miR-103a/107/107ab
                                       NM_130786 0.09
                              A1BG
```

-0.448

-0.448

-0.448

```
> dim(targetScanPCT)
[1] 2938804 4
```

3 TargetScore

Encouraged by the superior performance of TargetScore (manuscript in peer-review), we applied TargetScore to all of the transfection data above. For further exploring miRNA targetome and their associations, we enclose the targetScores results in this package.

```
> targetScoreMatrix <- get_precomputed_targetScores()</pre>
> head(names(targetScoreMatrix))
[1] "hsa-miR-34b"
                    "hsa-miR-34c" "hsa-miR-205" "hsa-miR-124" "hsa-miR-1"
[6] "hsa-miR-181a"
> head(targetScoreMatrix[[1]])
               logFC targetScanCS targetScanPCT targetScore
SGIP1
         0.077526011
                              0.00
                                                   0.03489650
AGBL4
         0.020639084
                              0.00
                                                0
                                                   0.03388637
NECAP2
         0.078650400
                              0.00
                                                0
                                                   0.03492518
CLIC4
         0.016043400
                             -0.03
                                                   0.24335149
        -0.002303429
                              0.00
                                                   0.03417828
ADC
                                                0
SLC45A1 -0.018655797
                              0.00
                                                   0.03457975
```

We can reproduce targetScores using the above data as demonstrated in the following example (require *TargetScore* package). As a convenience function, we applied a wrapper function called getTargetScores that does the following: (1) given a miRNA ID, obtain fold-change(s) from logFC.imputed matrix or use the user-supplied fold-changes; (2) retrives TargetScan context score (CS) and PCT (if found); (3) obtain validated targets from the local mirTarBase file; (4) compute targetScore. We apply getTargetScores function using miRNA hsa-miR-1, which we know has all three types of data, namely logFC, targetScan context score, and PCT.

```
> library(TargetScore)
> library(gplots)
> myTargetScores <- getTargetScores("hsa-miR-1", tol=1e-3, maxiter=200)
> table((myTargetScores$targetScore > 0.1), myTargetScores$validated) # a v
> # obtain all of targetScore for all of the 112 miRNA
>
> logFC.imputed <- get_precomputed_logFC()
> mirIDs <- unique(colnames(logFC.imputed))
> # takes time
> # targetScoreMatrix <- mclapply(mirIDs, getTargetScores)
> # targetScoreScoreScores
```

> # names(targetScoreMatrix) <- mirIDs

4 Session Info

```
> sessionInfo()
R version 4.2.1 (2022-06-23)
Platform: x86_64-pc-linux-qnu (64-bit)
Running under: Ubuntu 20.04.5 LTS
Matrix products: default
        /home/biocbuild/bbs-3.16-bioc/R/lib/libRblas.so
BLAS:
LAPACK: /home/biocbuild/bbs-3.16-bioc/R/lib/libRlapack.so
locale:
 [1] LC_CTYPE=en_US.UTF-8
                                LC_NUMERIC=C
 [3] LC TIME=en GB
                                LC COLLATE=C
 [5] LC_MONETARY=en_US.UTF-8
                                LC MESSAGES=en US.UTF-8
 [7] LC_PAPER=en_US.UTF-8
                                LC_NAME=C
 [9] LC_ADDRESS=C
                                LC_TELEPHONE=C
[11] LC MEASUREMENT=en US.UTF-8 LC IDENTIFICATION=C
attached base packages:
[1] stats
              graphics
                       grDevices utils datasets methods
                                                                 base
other attached packages:
[1] TargetScoreData_1.34.0
loaded via a namespace (and not attached):
[1] compiler_4.2.1 tools_4.2.1
```

References

Sean Davis and Paul S Meltzer. GEOquery: a bridge between the Gene Expression Omnibus (GEO) and BioConductor. *Bioinformatics* (Oxford, England), 23(14):1846–1847, July 2007.

Sheng-Da Hsu, Feng-Mao Lin, Wei-Yun Wu, Chao Liang, Wei-Chih Huang, Wen-Ling Chan, Wen-Ting Tsai, Goun-Zhou Chen, Chia-Jung Lee, Chih-Min Chiu, Chia-Hung Chien, Ming-Chia Wu, Chi-Ying Huang, Ann-Ping Tsou, and Hsien-Da Huang. miRTarBase: a database curates experimentally validated microRNA-target interactions. *Nucleic acids research*, 39 (Database issue):D163–9, January 2011.

O Troyanskaya, M Cantor, G Sherlock, P Brown, T Hastie, R Tibshirani, D Botstein, and R B Altman. Missing value estimation methods for DNA microarrays. *Bioinformatics (Oxford, England)*, 17(6):520–525, June 2001.