

Supplementary Tables

Selcen Arı

16 09 2019

Table S1: *minsamp* sample dataset that includes interaction factors.

competing	miRNA	Competing_expression	miRNA_expression	seed_type	region	energy
Gene1	Mir1	10000	1000	0.43	0.30	-20
Gene2	Mir1	10000	1000	0.43	0.01	-15
Gene3	Mir1	5000	1000	0.32	0.40	-14
Gene4	Mir1	10000	1000	0.23	0.50	-10
Gene4	Mir2	10000	2000	0.35	0.90	-12
Gene5	Mir2	5000	2000	0.05	0.40	-11
Gene6	Mir2	10000	2000	0.01	0.80	-25

Note: Energy values in miRNA:target pairs are represented by high-throughput studies (Helwak et al. 2013; Moore et al. 2015) which are utilized in this study. On the other hand, we have specified the other interaction factors, seed type and location of binding region on the target, as numeric values based on the previous studies.(Grimson et al. 2007) have compared the seed types' effect on target repression with few miRNA had canonical seed pairing in their study. Additionally, (Bartel 2009) and (Betel et al. 2010) have studied on functional and non-functional seed interactions. Based on results of these studies we have arranged seed types of miRNA:target interactions as numeric values. We also have redefined location of binding region on the target as numeric values, based on studies of (Hausser et al. 2013) and (Helwak et al. 2013). With this process, we have handled this entegrated dataset in context of competitor behaviours and functionality of interactions.

Table S2: Efficiency factors for seed types.

	seed_type	seed_type_effect
1	6-mer_noncanonical	0.05
2	9-mer	0.43
3	6-mer	0.07
4	8-mer	0.43
5	7-mer	0.23
6	none	0.01
7	5-mer_noncanonical	0.04
8	5-mer	0.05
9	6-merA1_noncanonical	0.05
10	7-mer-8m_noncanonical	0.21
11	7-mer-8m	0.25
12	8-mer_noncanonical	0.35
13	7-merA1_noncanonical	0.16
14	7-merA1	0.19
15	6-merA1	0.07

Table S3: Efficiency factors for binding regions on targets

	region	region_effect
1	3UTR	0.84
2	CDS	0.42
3	3UTRCDS	0.93
4	5UTR	0.01
5	5UTRCDS	0.42
6		0.01
7	intron	0.01
8	CDS3UTR	0.93
9	CDS5UTR	0.42
10	exon_unclassified	0.20
11	CDS3UTRintron	0.93
12	3UTRintron	0.84
13	CDSintron	0.42
14	5UTRintron	0.01
15	5UTR3UTR	0.93
16	CDS5UTR3UTR	0.93

Table S4: Example of E9GE_mirnagenormal dataset.

Hugo_Symbol	miRNA_name	mirna_RPM	GE_normal	energy	seed_type_effect	region_effect
ENAH	hsa-let-7a-5p	111204.15	7540	-22.70	0.01	0.00
GALNT2	hsa-let-7a-5p	111204.15	2824	-20.50	0.14	0.00
RLF	hsa-let-7a-5p	111204.15	1144	-18.00	0.03	0.20
MAST2	hsa-let-7a-5p	111204.15	2640	-22.60	0.24	0.00
DOCK1	hsa-let-7a-5p	111204.15	4826	-20.50	0.01	0.00
ZBTB16	hsa-let-7a-5p	111204.15	315	-24.30	0.14	0.00

As a result of simulation a dataset, a graph object is obtained that includes various variables in edge and node data. A graph object includes variables at followings.

Table S5: The context graph object during the process.

Variables	Structure	Means
Node Variables		
name	character	node name
type	character	Competing or miRNA
node_id	numeric	in on graph object
initial_count	numeric	Initial Expression value of node
count_pre	numeric	Expression value of node at previous regulation
count_current	numeric	Existing expression value of node
changes_variable	character	Regulation of node (Up, down or steady)
Edge Variables		
Competing name	character	name of genes
miRNA name	character	name of miRNAs
Competing expression	numeric	Expression values of competing elements at steady-state
miRNA expression	numeric	Expression values of miRNA elements at steady-state
energy	numeric	coefficient of miRNA:target interactions (binding affinity)
seed type	numeric	coefficient of miRNA:target interactions (binding affinity)

Variables	Structure	Means
<code>mirna_count</code>	numeric	<code>_pre</code> : miRNA expression at previous iteration; <code>_current</code> : miRNA expression at present iteration
<code>effect</code>	numeric	<code>_pre</code> : total miRNA repressive effect on individual target at previous iteration ; <code>_current</code> : miRNA repressive effect on individual target at present iteration
<code>effect_list</code>	list	list of miRNA repressive effect on individual target for each iteration

REFERENCES

- Bartel, David P. 2009. "MicroRNAs: Target Recognition and Regulatory Functions." *Cell* 136 (2): 215–33. <https://doi.org/10.1016/j.cell.2009.01.002>.
- Betel, Doron, Anjali Koppal, Phaedra Agius, Chris Sander, and Christina Leslie. 2010. "Comprehensive Modeling of microRNA Targets Predicts Functional Non-Conserved and Non-Canonical Sites." *Genome Biology* 11 (8): R90.
- Grimson, Andrew, Kyle Kai-How Farh, Wendy K. Johnston, Philip Garrett-Engele, Lee P. Lim, and David P. Bartel. 2007. "MicroRNA Targeting Specificity in Mammals: Determinants Beyond Seed Pairing." *Molecular Cell* 27 (1): 91–105. <https://doi.org/10.1016/j.molcel.2007.06.017>.
- Hausser, J., A. P. Syed, B. Bilen, and M. Zavolan. 2013. "Analysis of CDS-Located miRNA Target Sites Suggests That They Can Effectively Inhibit Translation." *Genome Research* 23 (4): 604–15. <https://doi.org/10.1101/gr.139758.112>.
- Helwak, Aleksandra, Grzegorz Kudla, Tatiana Dudnakova, and David Tollervey. 2013. "Mapping the Human miRNA Interactome by CLASH Reveals Frequent Noncanonical Binding." *Cell* 153 (3): 654–65. <https://doi.org/10.1016/j.cell.2013.03.043>.
- Moore, Michael J., Troels K. H. Scheel, Joseph M. Luna, Christopher Y. Park, John J. Fak, Eiko Nishiuchi, Charles M. Rice, and Robert B. Darnell. 2015. "miRNA-Target Chimeras Reveal miRNA 3'-End Pairing as a Major Determinant of Argonaute Target Specificity." *Nature Communications* 6 (November): 8864. <https://doi.org/10.1038/ncomms9864>.