

Supplementary Materials for
“A web server for designing molecular switches composed of
two interacting RNAs”

Akito Taneda and Kengo Sato

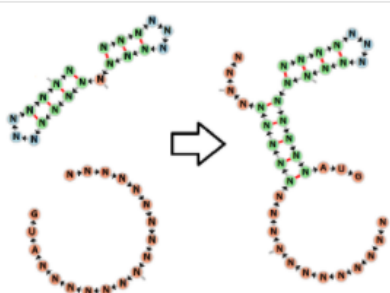
MODENA web server About References Download benchmark target structures Help

MODENA web server

Multi-objective design of RNA switches and structured RNA sequences. MODENA utilizes multi-objective optimization and RNA secondary structure prediction for computational RNA design.

[More Info](#)

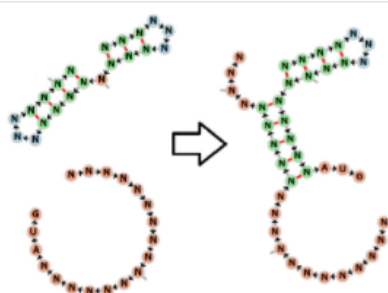
Design templates



RNA-RNA interaction switch (RactIP)

This designs two RNA sequences that fold into a user-prescribed target JOINT structure. In addition, the user can specify target structures for single RNAs. An external pseudoknot (including a kissing-hairpin) is allowed (whereas pseudoknots within each sequence are not allowed).

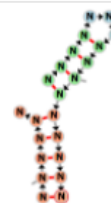
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RNA-RNA interaction switch (RNAcofold)

This designs two RNA sequences that fold into a user-prescribed target JOINT structure. In addition, the user can specify target structures for single RNAs. Any pseudoknotted joint secondary structure is not allowed.

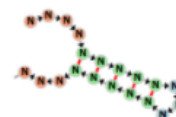
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Interacting two RNAs

This designs two RNA sequences that fold into a user-prescribed target JOINT secondary structure. An external pseudoknot is allowed (whereas pseudoknots within each sequence are not allowed)

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Inverse folding of a single RNA

This designs a single RNA sequence that folds into a user-prescribed target secondary structure.

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Figure S1. The top page of MODENA web server.

Designing RNA-RNA interaction switch

This design explores the sequence space to find RNA sequences that fold into the target structures in silico.

This design uses RactIP to predict secondary structures.

An external pseudoknot (eg an intermolecular pseudoknot including a kissing-hairpin) is allowed (whereas pseudoknots within each sequence is not allowed).

Examples of runtimes can be browsed [here](#).

Current limit of this server is ≥ 20 nt and ≤ 230 nt. If you use this web server, please cite [these papers](#).

Step 1: Input your targets to the following form in [S+ notation](#) :

(If you would like to directly specify the targets in the standard dot-bracket notation, you can skip Step 1 & 2 and go to Step3).

Line 1: The target joint structure of two RNAs

Line 2: Two target structures (for two single RNAs)

Using structure constraints of RactIP, intermolecular base pair formation is prohibited to predict the structure of the two single RNAs

Line 3 and more lines (optional) : structure and/or sequence motifs

```
U3 (15 [15 U6 ] & U15 (15 U6 ] ) U10
U3 (15 U2 (2 U12 ) U3 ) & U15 (15 U21 ) U10
```

Step 2: Click the above button to automatically generate your target(s) and sequence constraints in the standard dot-bracket notation; the generated structures and constraints are displayed in the form shown below.

Step 3: Confirm (or input) your targets in the following form (the targets are written in the standard dot-bracket notation [$*?+$ are also allowed]):

Line 1: The target joint secondary structure of two RNAs

Line 2: Two target secondary structures (for two single RNAs)

Line 3: Sequence constraints

```
... (((((((((((((((([[[[[[[[[[[[.....))))))))))))))&..... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))).....
... (((((((((((((((([[[[[[[[[[[[.....))))))))))))))&..... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))).....
#####
```

The central value of desired G+C content (%): The half-range of the allowed G+C content (%):

GA population size:

Initial random number:

Prohibited sequence motifs (if multiple motifs are specified, please concatenate them with comma.):

Prohibited polynucleotide tracts. Those with the length (in nucleotides) longer than the value specified here are prohibited:

PolyA tract is: PolyC tract is: PolyG tract is: PolyU tract is:

Step 4: Click the next button to submit your design!

Figure S2. The submission page of RNA-RNA switch design in MODENA web server.

Design result

No.	Str.dist.	Ene.Diff.	Seed	G+C(%)	Designed sequences & structures predicted by RactIP (free energies in kcal/mol)
1	0.00	19.61	-5.83	58.78	<pre> ... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] AUGGCGAAUAGCGGAUCCGGGCCUGCCUUCUCCUGCACAGGAUCCGCUAUUCGC/GUGACCUCUGUUAAGCCACGCUAUGGCGCUAUUUCGGAGAGGCGAGGCC ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] Tract>3nt= 0 Constr= 0 tractType= ACGU The G+C content is within the prescribed range, and no prohibited motif (if prescribed) is included in th /// Post-processing result. The following values were obtained after the optimization has been done. /// 0.00 :Free energy value of unfavored seed for the homodimer of sequence 1 -0.75 :Free energy value of unfavored seed for the homodimer of sequence 2 </pre> <p>draw by forna</p>
2	0.00	20.01	-5.83	58.02	<pre> ... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] AUGGUGGGUAAAGGGCUUAGGGCCUGCCUUCUCCUGCACAAUAGCCUUUACCCAC/GUGACCUCUGUUAAGCCACCUACGGCGCUAUUUCGGAGAGGCGAGGCC ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] </pre> <p>draw by forna</p>
3	0.00	20.45	-5.83	58.78	<pre> ... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ACACCGAAUAGGGCUUAGGGCCUGCCUUCUCCUGCUAGUAAGCCUUUAVUCGG/AGCAUAGCCACAAUGGGCCACCUACGGCGCUAGUUCGGAGAGGCGAGGCC ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] </pre> <p>draw by forna</p>
4	0.00	20.45	-5.83	58.78	<pre> ... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ACACCGAAUAGGGCUUAGGGCCUGCCUUCUCCUGCUAGUAAGCCUUUAVUCGG/AGCAUAGCCACAAUGGGCCACCUACGGCGCUAGUUCGGAGAGGCGAGGCC ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] </pre> <p>draw by forna</p>
5	2.00	21.87	-6.90	58.78	<pre> ... (((((((((((((((([[[[[[[[[[[[.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] AUGGUGGGUAAAGGGUCCGGGCCUGCCUUCUCCUGCACAGGACCCUUUACCCAC/GUGACCUCUGUUAAGCCACGCUAUGGCGCUAUUUCGGAGAGGCGAGGCC ... (((((((((((((((((.....)))))))))))))))/..... (((((((((((((((.....]]]]]]]]]]]]]]]]]]]] </pre> <p>draw by forna</p>

Figure S3. An example of the result page output from MODENA web server.