

Supplement contents:

This file:

- **supplement_contents.pdf**

Python script for modeling tRNAs:

- **modeling.py:** a script that does all the modeling mentioned in the article. To run the script one must have Python (<http://www.python.org/>) and ModeRNA (<http://genesilico.pl/moderna/>) installed, as well as all input files (see below) present in the same directory as the script. Then, it is sufficient to type in the terminal: *python modeling.py*

Alignments:

- **target.fasta:** target sequence (*E. coli* tRNA^{Thr}) taken from file 1QF6.pdb.
- **target_1EHZ.fasta:** alignment between target sequence and the sequence of *S. cerevisiae* tRNA^{Phe} (PDB code: 1EHZ, chain A).
- **target_1C0A.fasta:** alignment between target sequence and the sequence of *E. coli* tRNA^{Asp} (PDB code: 1C0A, chain B).

Templates for modeling:

- **1EHZ.pdb:** 3D structure of *S. cerevisiae* tRNA^{Phe}, original file downloaded from PDB.
- **1C0A.pdb:** 3D structure of *E. coli* tRNA^{Asp}, original file downloaded from PDB.

Models:

All models provided by us are located in directory called “models”.

- **model_1EHZ_superimposed.pdb:** model obtained with the automatic modeling procedure on the yeast tRNA^{Phe} (1EHZ, chain A) template superimposed on the original structure of *E. coli* tRNA^{Thr} (1QF6).
- **model_1C0A_superimposed.pdb:** model obtained with the automatic modeling procedure on the *E. coli* tRNA^{Asp} (1C0A, chain B) template superimposed on the original structure of *E. coli* tRNA^{Thr} (1QF6).
- **model_1EHZ_insertion_9nt_superimposed.pdb:** model obtained with the advanced modeling procedure on the two templates: yeast tRNA^{Phe} (1EHZ, chain A) – overall structure, and *E. coli* tRNA^{Asp} (1C0A, chain B) – anticodon 9nt insertion. The model is superimposed on the original structure of *E. coli* tRNA^{Thr} (1QF6).
- **model_1EHZ_insertion_15nt_superimposed.pdb:** model obtained with the advanced modeling procedure on the two templates: yeast tRNA^{Phe} (1EHZ, chain A) –

overall structure, and *E. coli* tRNA^{Asp} (1C0A, chain B) – anticodon 15nt insertion. The model is superimposed on the original structure of *E. coli* tRNA^{Thr} (1QF6).

- **model_1EHZ_insertion_19nt_superimposed.pdb:** model obtained with the advanced modeling procedure on the two templates: yeast tRNA^{Phe} (1EHZ, chain A) – overall structure, and *E. coli* tRNA^{Asp} (1C0A, chain B) – anticodon 19nt insertion. The model is superimposed on the original structure of *E. coli* tRNA^{Thr} (1QF6).

Reference structure:

- **1QF6.pdb:** original (solved experimentally) structure of *E. coli* tRNA^{Thr} (chain B) in the complex with an aminoacyl-tRNA synthetase (aaRS) (chain A).