Trajectories of CopA-CopT under the "CPU microscope"

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universität wien

TBI

FWF
Der Wissenschaftsfonds.

Motivation

[1]

[1] Figure modified from: https://www.clipartmax.com

Motivation

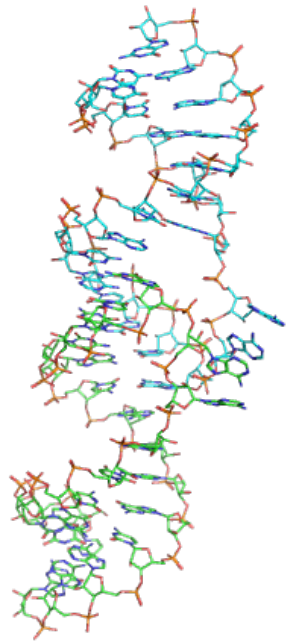
[1]

[1] Figure modified from: https://www.clipartmax.com

3D Representation - The microscope

All atom Simulations[1]

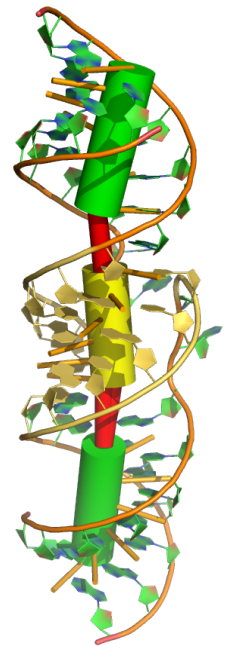
AMBER
CHARM
FARNA/FARFAR
...



PDB - Crystal[2,3]

Coarse-grained Approaches[1]

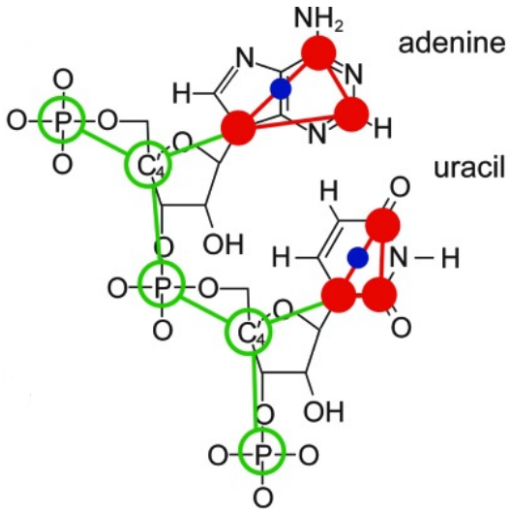
ERNWIN
Kinefold
SimRNA
...



Ernwin[2,3,4]

[1] Dawson, W. K. et al.(2016) Methods
[2] Ennifar, E. et al.(2006) J.Mol.Biol.
[3] Visualized via Pymol: The PyMOL Molecular Graphics System, Version 2.0 Schrödinger, LLC.
[4] Ernwin calculation: Kerpedjiev, P. et al.(2015) RNA

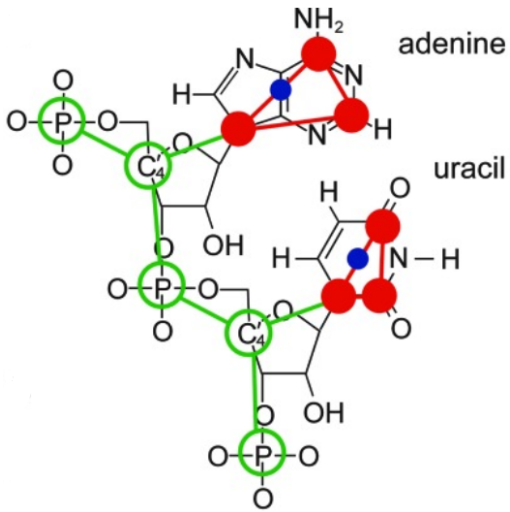
SimRNA - The microscope's features



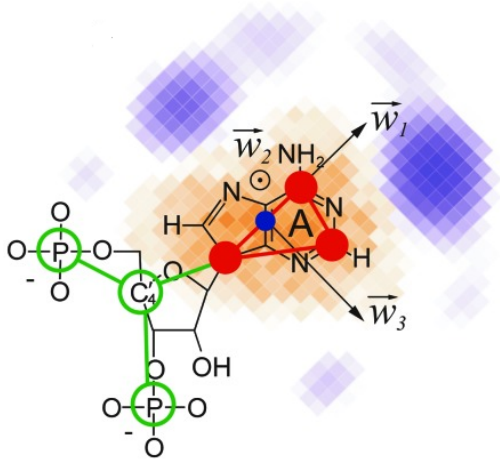
[1]

- Backbone: P, C4
- Bases: Pyrimidines: N1, C2, C4
  Purine: N9, C2, C6
- Midpoint of each base

SimRNA - The microscope's features



[1]



[1]

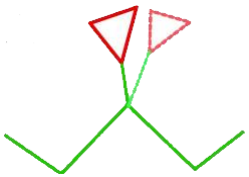
- Backbone: P, C4
- Bases: Pyrimidines: N1, C2, C4
  Purine: N9, C2, C6
- Midpoint of each base

3D cubic grid

[1] Figures modified from: Boniecki, M. J. et al.(2015) Nucleic Acids Research

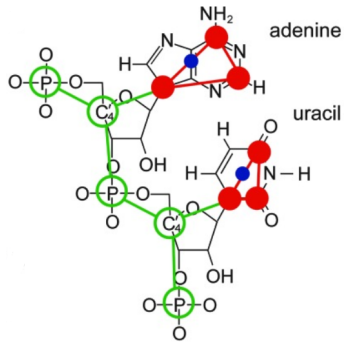
SimRNA - The microscope's features

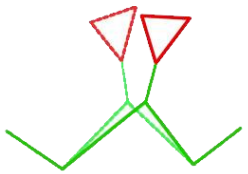
[1]



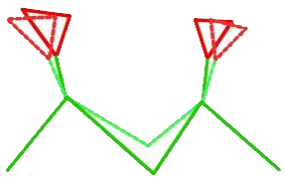
Change the Position of . . .

. . . the base

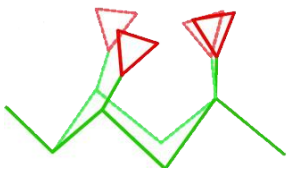




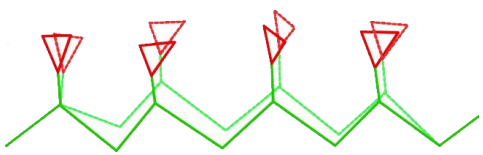
. . . the backbone (C4)



. . . the backbone (P)



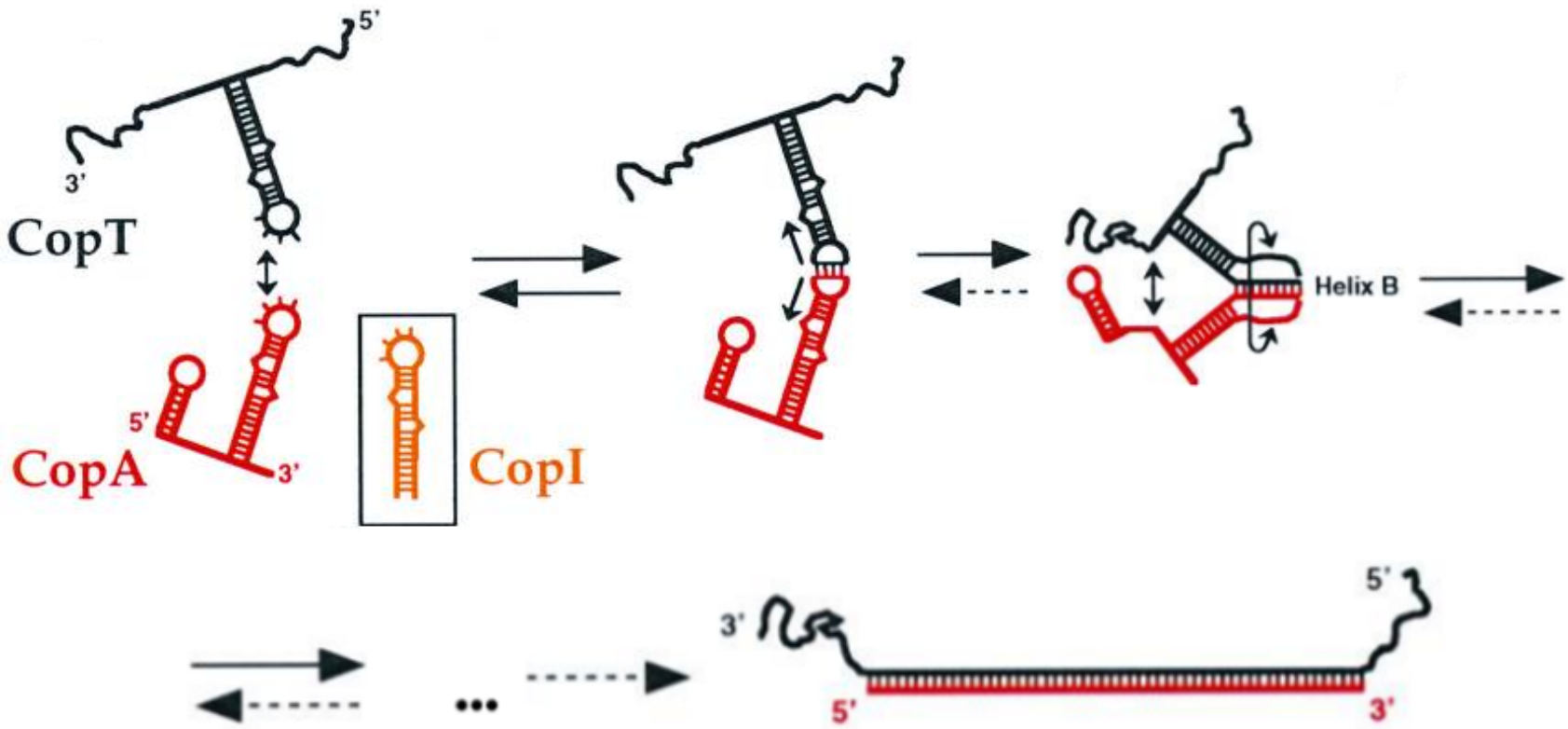
. . . two subsequent atoms of the backbone



Change the direction of a backbone's fragment

[1] Figures modified from: Boniecki, M. J. et al.(2015) Nucleic Acids Research

Model: CopA-CopT / CopI-CopT



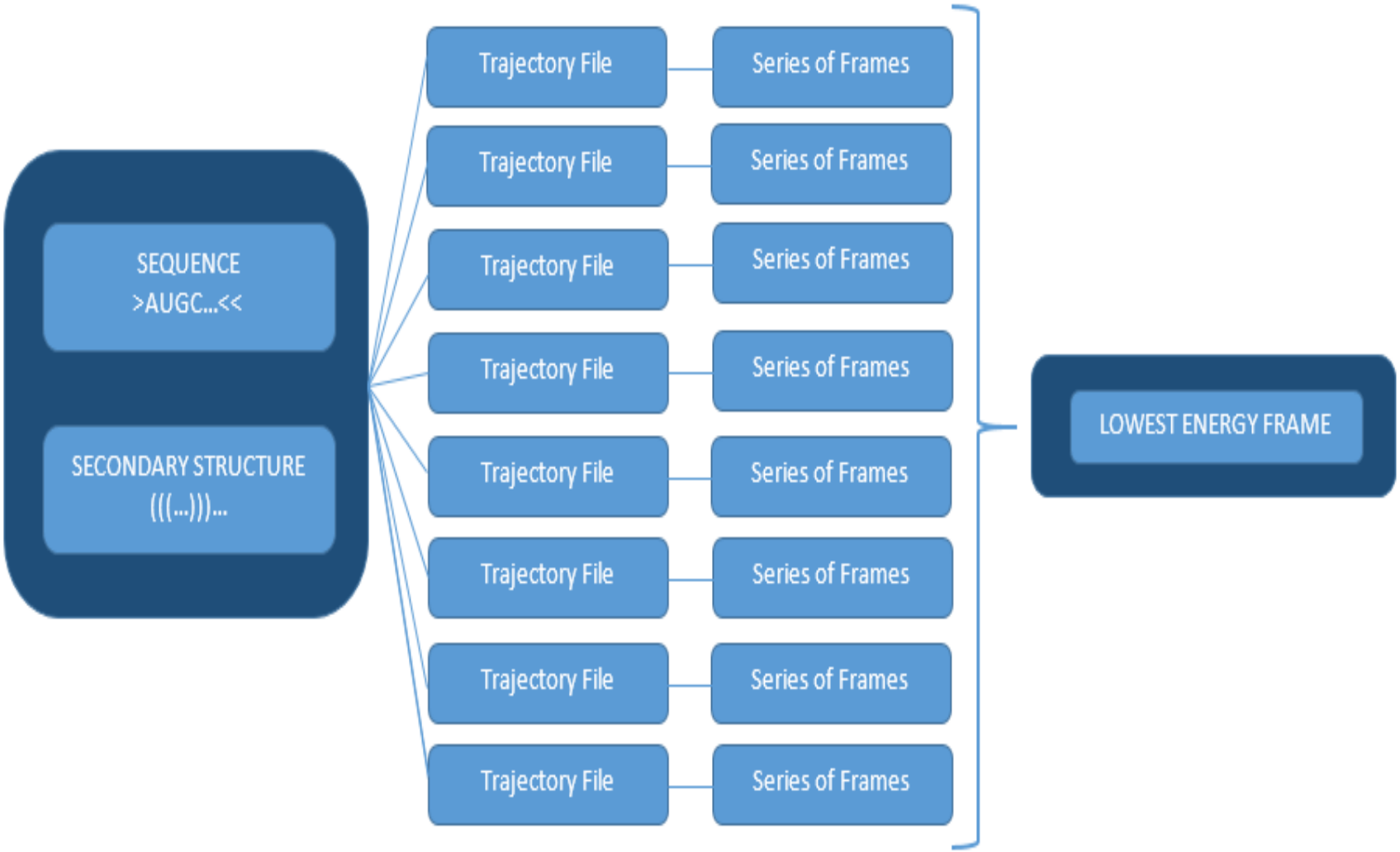
[1]

[1] Figures modified from: Kolb, F. A.et al. (2000) NThe EMBO Journal

Input

```
CCCCUUUAAAACCCCGGGG GGGGAAAUUUUCCCCCCCC
((((............))))  ((((............))))
.......(((.........  .......))))........
```

Pathway

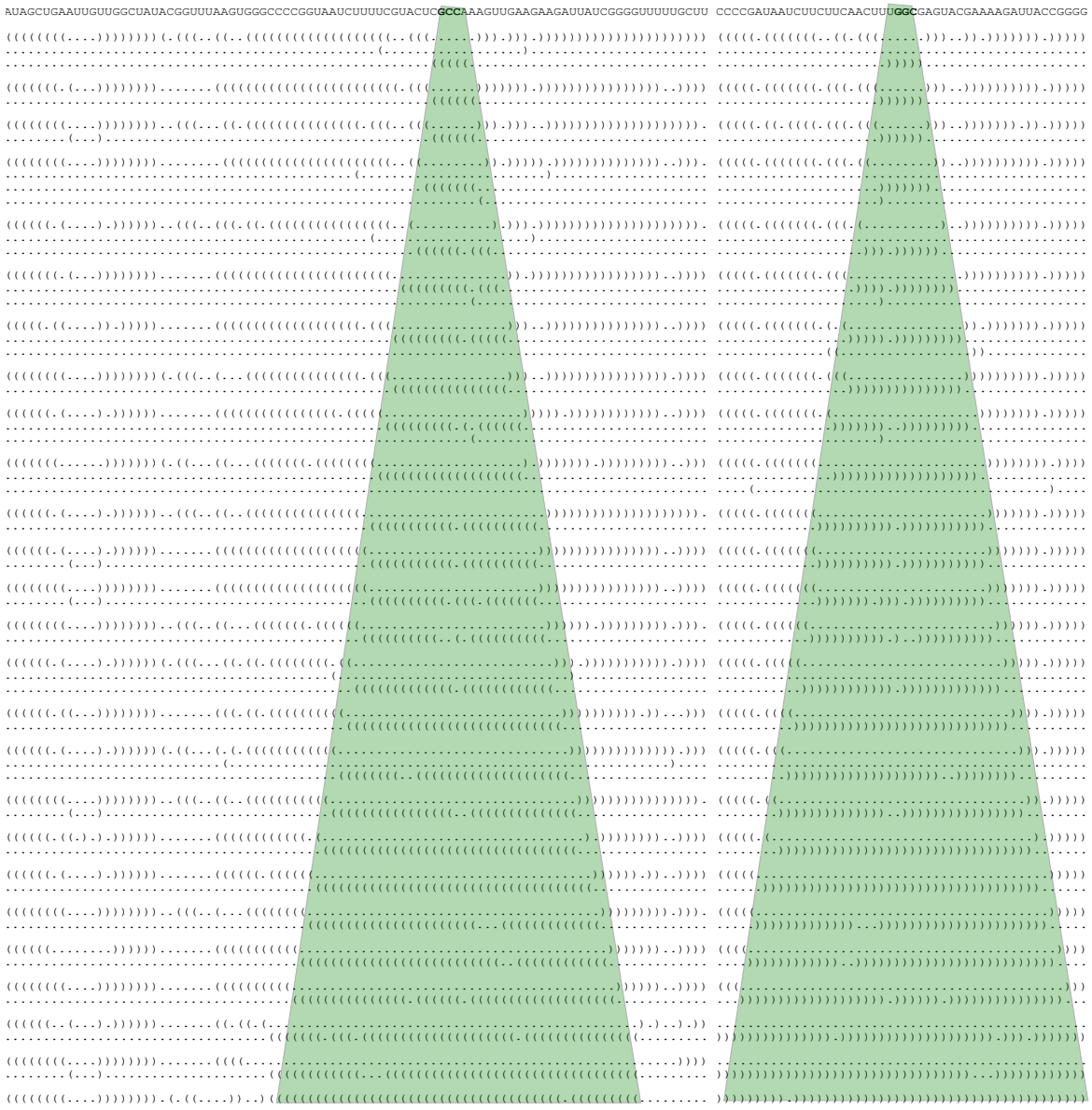


[1]

[1] Partially based on: Boniecki, M. J. et al.(2015) Nucleic Acids Research

CopI-CopT: Input

CopI-CopT: Output



Output

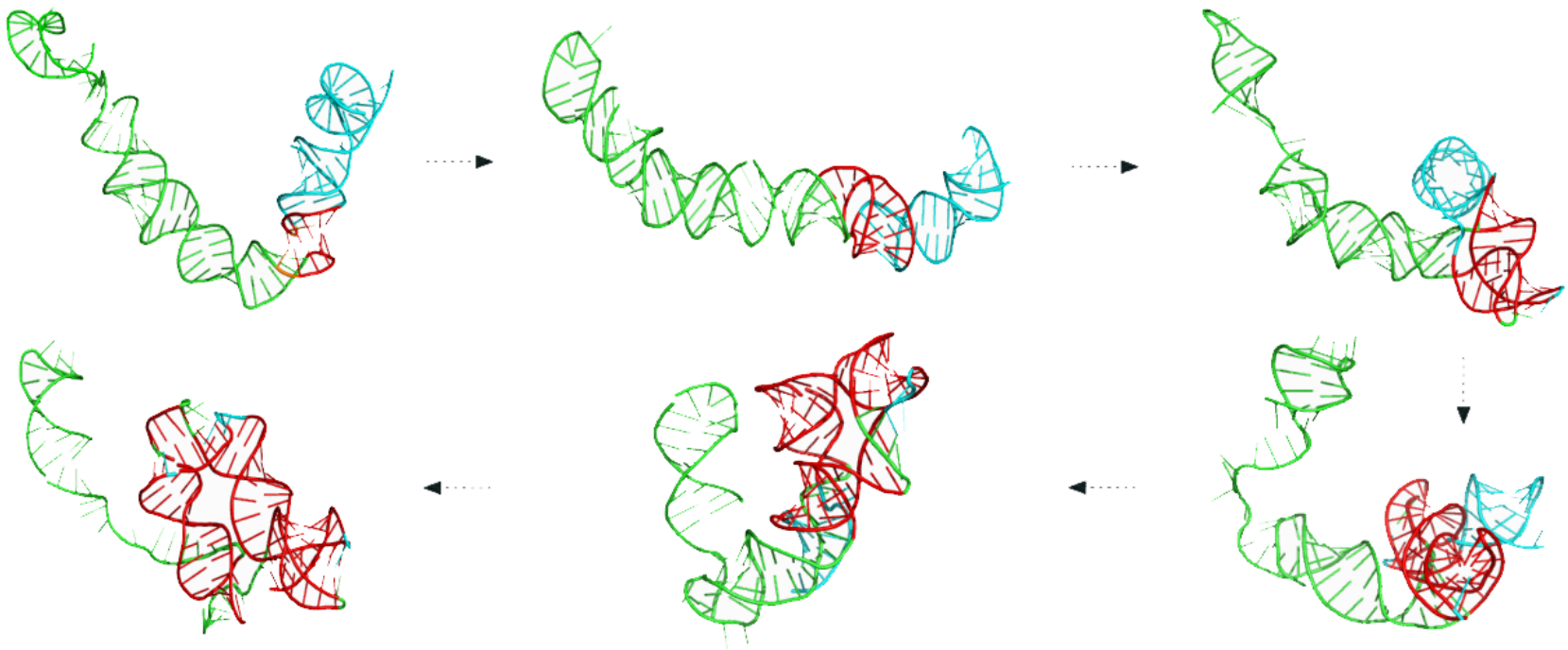
Multiplets:

```
CUUUUCGUACUCGCCAAAGUUGAAGAAG UCUUCAACUUUGGCGAGUACGAAA
((((((..(((......))).))).)))  (..((.(((......))).)).)
....(..................)....  ........................
..........((((.........  .........))))..........
```

Bulges:

```
CUCGUACUCGCCAAAGUUGAAGAAG CUUCUUCAACUUUGGCGAGUACGAG
((....................))  ((....................))
..(((((((..(.((((((((((..  ..))))))))))).)..)))))))..
```

Cutouts of the predicted binding pathway of CopI-CopT



CopT
Interaction Site
CopI
Multiplet

Trajectories calculated via SimRNA: Boniecki, M. J. et al.(2015) Nucleic Acids Research
Visualized via Pymol: The PyMOL Molecular Graphics System, Version 2.0 Schrödinger, LLC.

Acknowledgements

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