RNA secondary structure visualized in Galaxy

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reminder: RNA function

RNA Functions

mRNA: translated to/encodes proteins
rRNA: ribosomal RNA, part of the ribosomes where the mRNA is translated
tRNA: “reads” the code of the mRNA and delivers the correct amino acid for the prolongation of the peptides

small RNA: especially in eukaryotes, many small RNA fragments are incorporated in RNA-binding proteins complexes or act as ribozymes, regulatory function

reminder: RNA primary structure

Primary Structure

GGGCGUGUGGCGUAGUUGGUAGCGCGCUCCCUUAGCAUGGGAGAGGUCAUCGGUU
CGAUUCCGGUCUCGUCCA

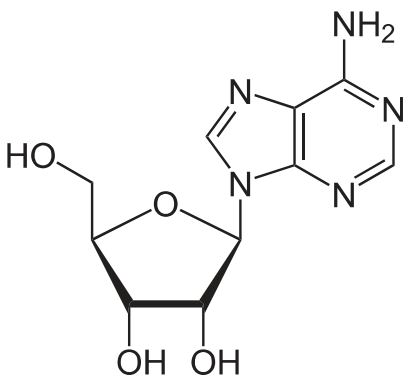
reminder: RNA primary structure

Primary Structure

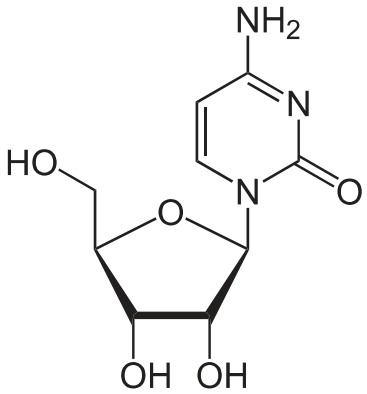
GGGCGUGUGGCGUAGUUGGUAGCGCGCUCCCUUAGCAUGGGAGAGGUCAUCGGUU
CGAUUCCGGUCUCGUCCA

Ribonucleosides

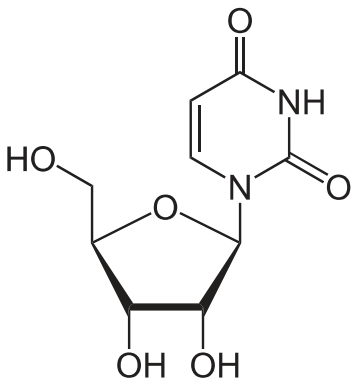
Adenosine



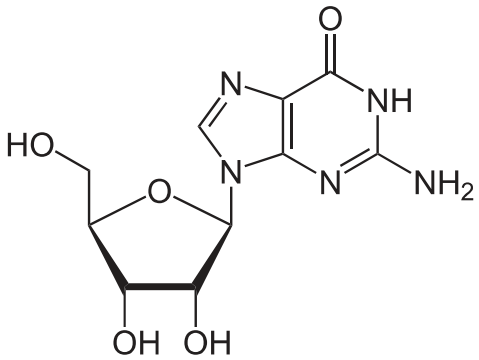
Cytidine



Uridine



Guanosine



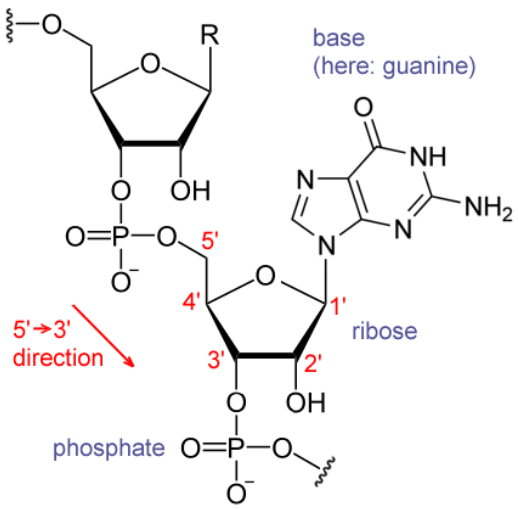
reminder: RNA primary structure

Primary Structure

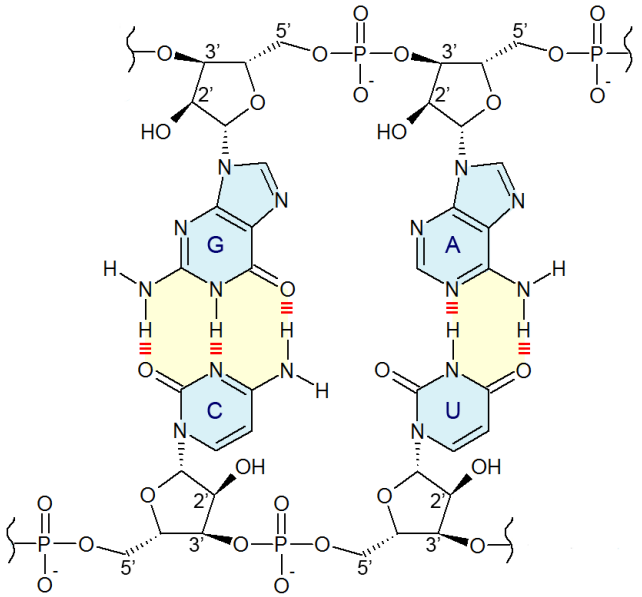
GGGCGUGUGGCGUAGUUGGUAGCGCGCUCCCUUAGCAUGGGAGAGGUCAUCGGUU
CGAUUCCGGUCUCGUCCA

Bonds

Phosphodiester bond
covalent



Hydrogen bonds
can form in a single strand of RNA
non-covalent



reminder: RNA secondary structure

Secondary structure

```
GGGCGUGUGGCGUAGUUGGUAGCGCGCUCCCUUAGCAUGGGAGAGGUCAUCGGUUCGAUUCCGGUCUCGUCCA
((((((((.((.......)).)))))))).......((((.(((...((((((.......))))))))).))))
```

reminder: RNA secondary structure

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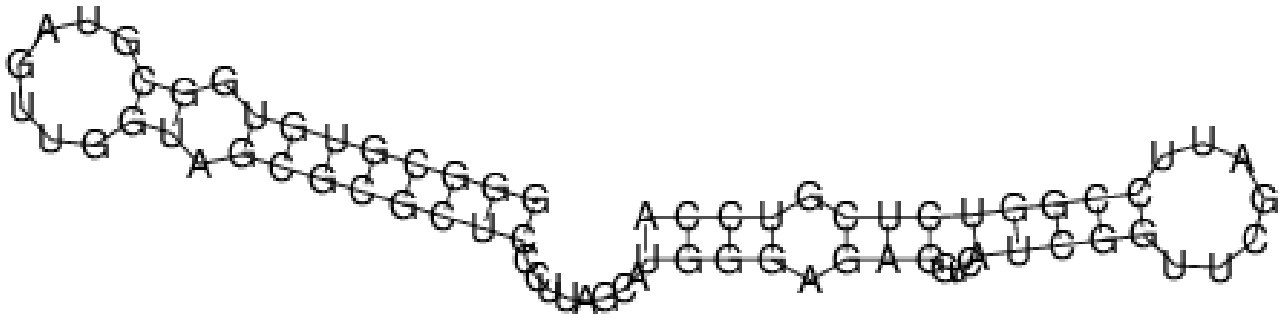

visualize RNA secondary structure

Secondary structure

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GGGCGUGUGGCGUAGUUGGUAGCGCGCUCCCUUAGCAUGGGAGAGGUCAUCGGUUCGAUUCCGGUCUCGUCCA
((((((((.((.....)).)))))))).........((((.(((...((((((.......)))))))))).))))
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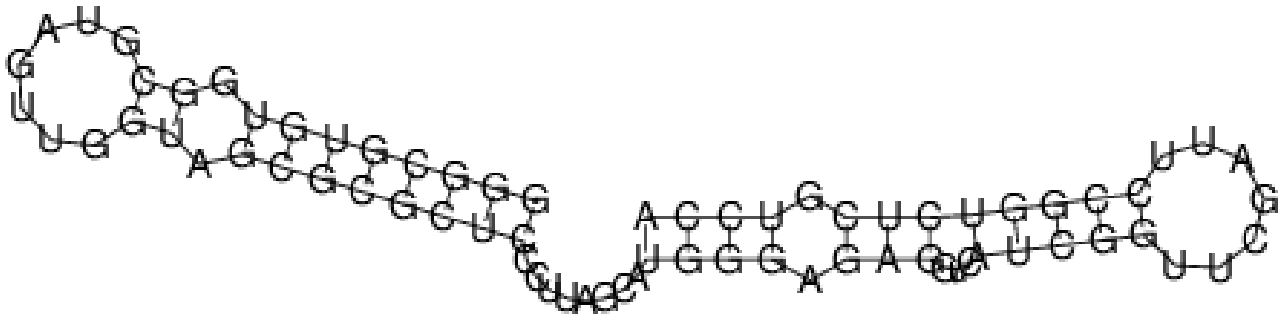

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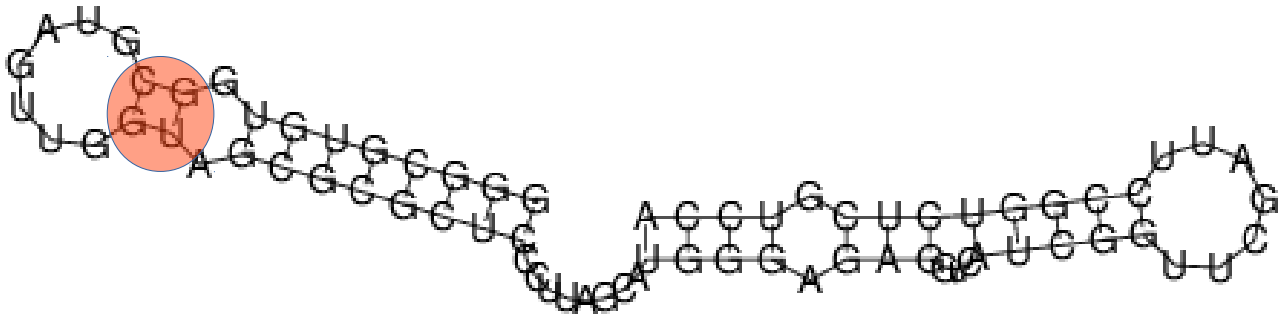

calculate RNA secondary structure

Secondary structure

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((((((((.((.......)).)))))))).......((((.(((...((((((.......))))))))).))))
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Algorithms by Zuker[1]

- Minimum Free Energy structure

calculate RNA secondary structure

Secondary structure

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- Minimum Free Energy structure
- Base Pairing Probability

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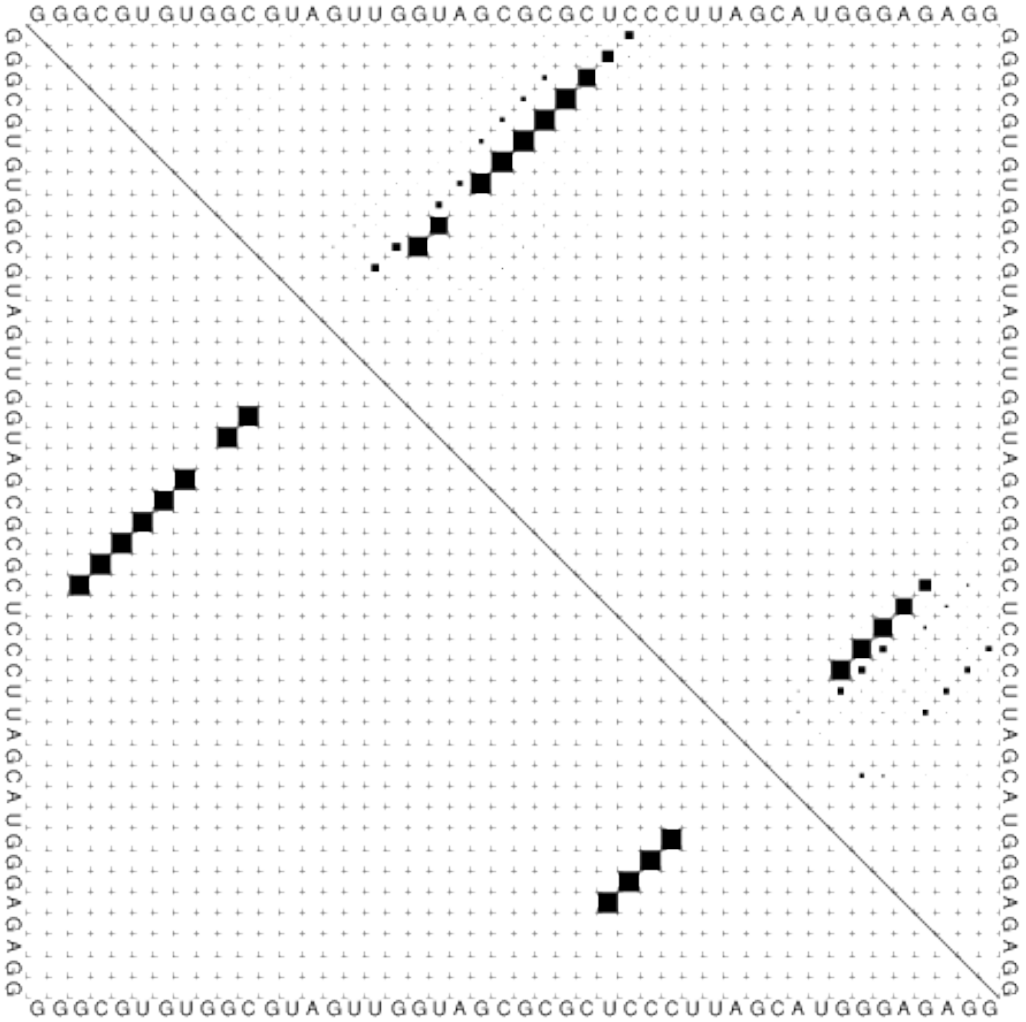
with RNAfold (ViennaRNA package)



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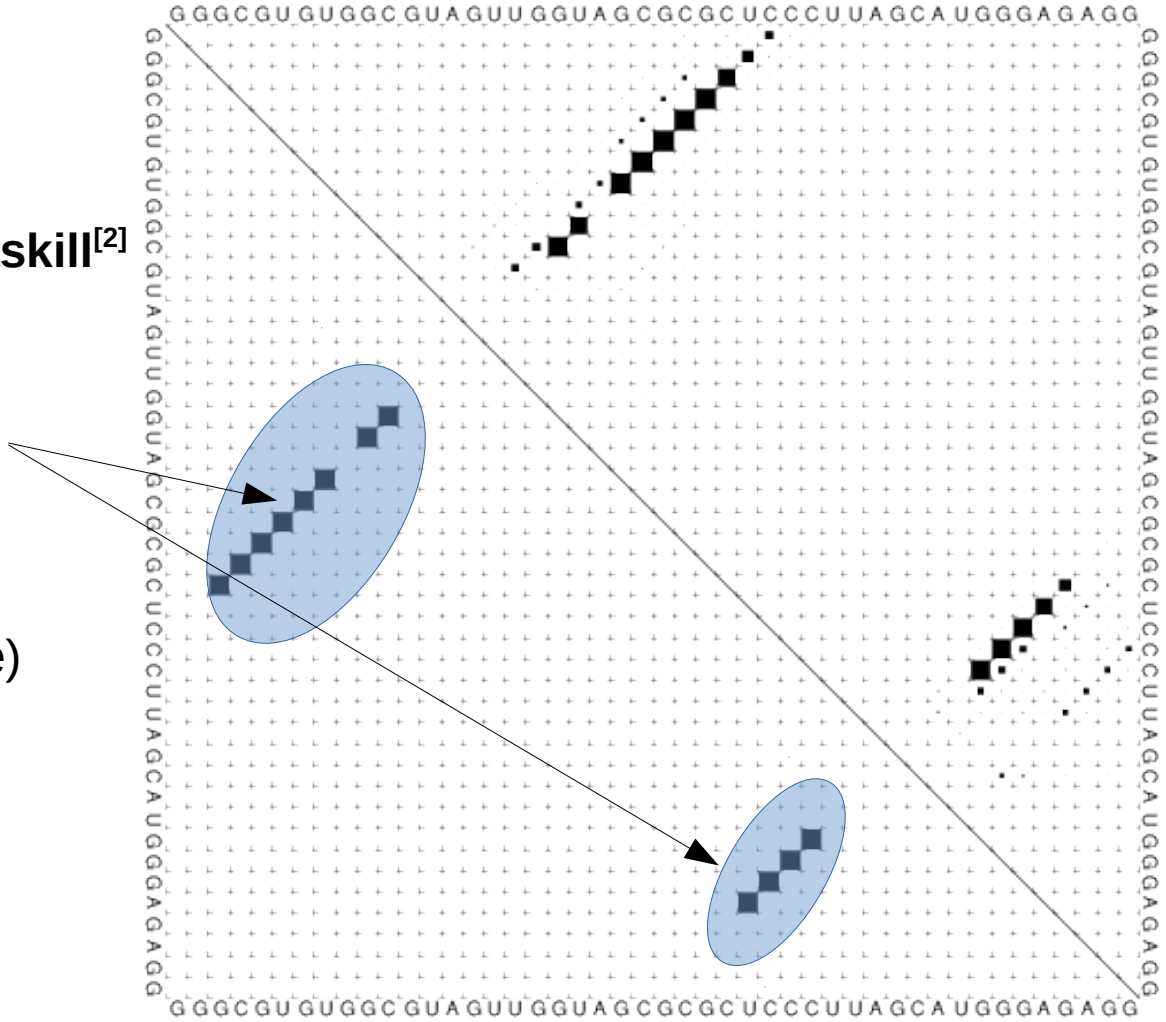

calculate RNA secondary structure

Secondary structure

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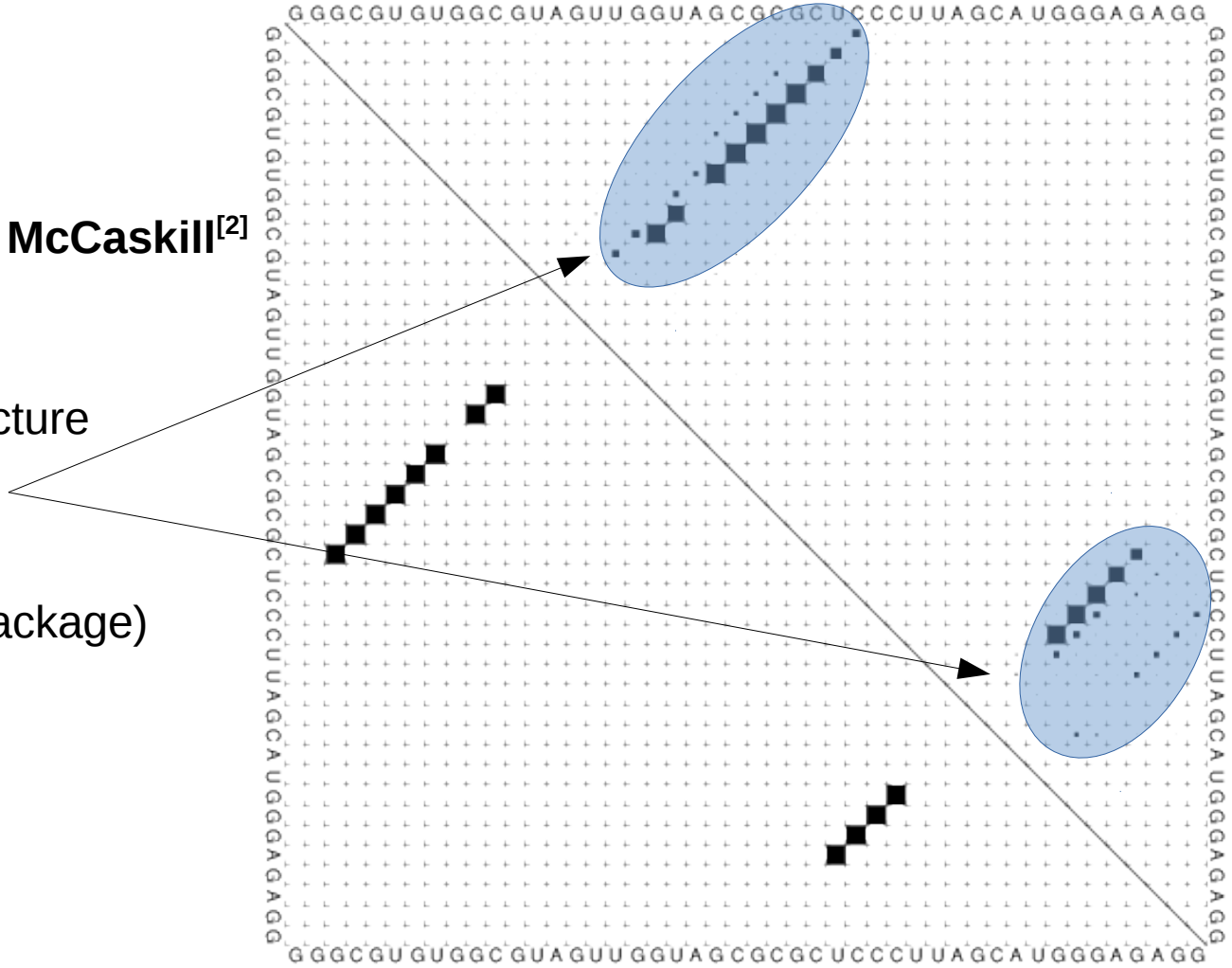

calculate RNA secondary structure

Secondary structure

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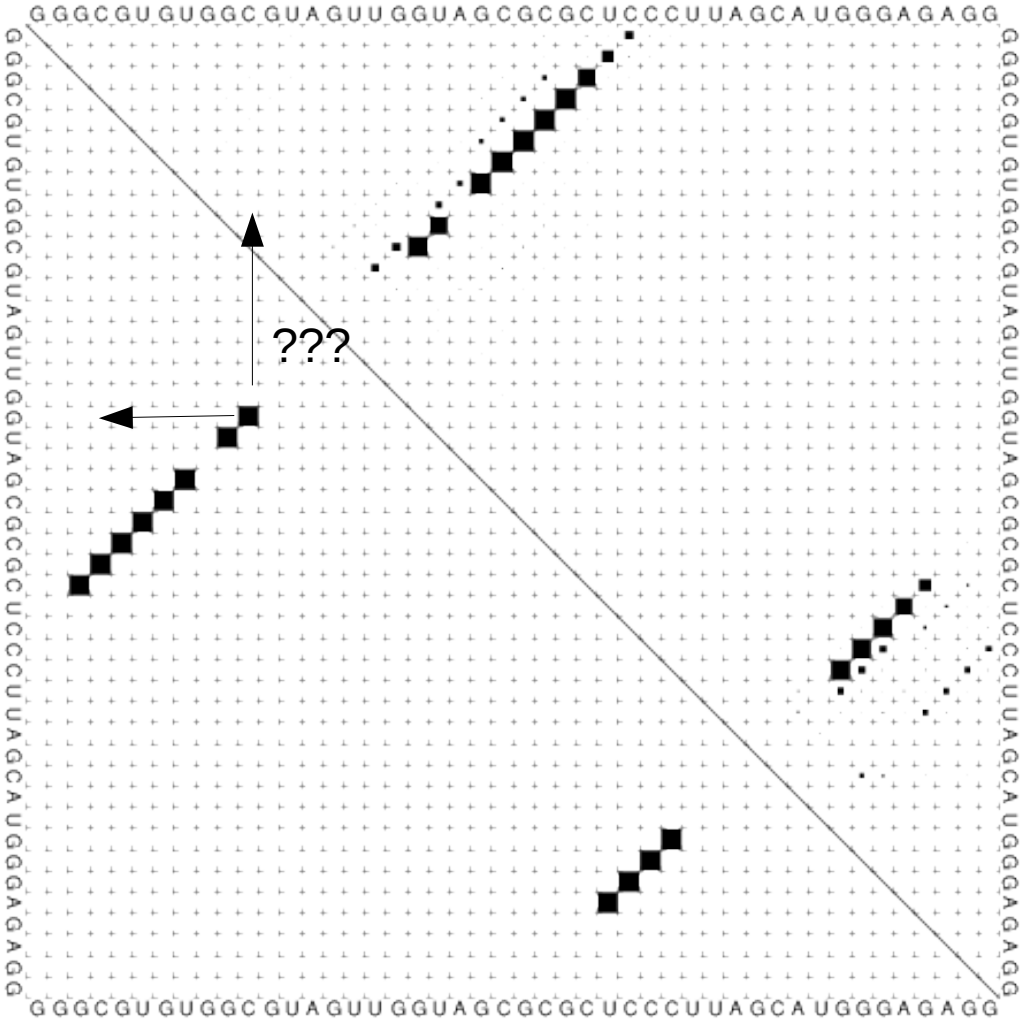

demo

Secondary structure

```
GGGCGUGUGGCGUAGUUGGUAGCGCGCUCCCUUAGCAUGGGAGAGGUCAUCGGUUCGAUUCCGGUCUCGUCCA
((((((((.((.......)).)))))))).......((((.(((...((((((.......))))))))).)))))
```

http://localhost:8080

Galaxy + Javascript libraries

Galaxy's visualization interface

galaxydir/config/plugins/visualizations

easy to test, easy to deploy, extensible
→ merge two views into one making them interact
→ breakable hydrogen bonds in the dotplot or by pulling strands apart
→ different potentials for the different bonds
→ add a datatype just for RNA secondary structures

```
>comment
GGUUAACUAGCC
((..(..)..))
```

D3 – Data Driven Documents

http://d3js.org/

Connect data with visible elements easily.

thank you !!

Literature

[1] M. Zuker, P. Stiegler (1981), "Optimal computer folding of large RNA sequences using thermodynamic and auxiliary information", Nucl Acid Res: 9, pp 133-148

[2] J.S. McCaskill (1990), "The equilibrium partition function and base pair binding probabilities for RNA secondary structures", Biopolymers: 29, pp 1105-1119

Images

Wikipedia

Repository

https://github.com/bgruening/galaxytools

- folder “visualizations”