Visualization of quadruplex structures

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Quadruplexes

- Quadruplexes are structural motifs of RNA, DNA and nucleic acid analogs
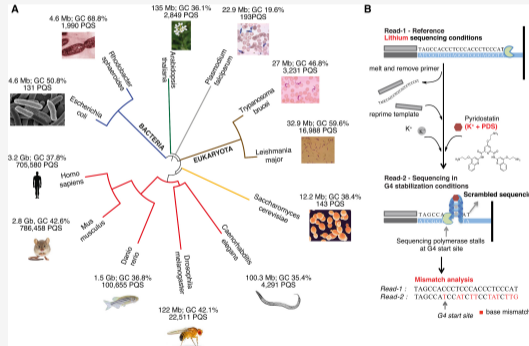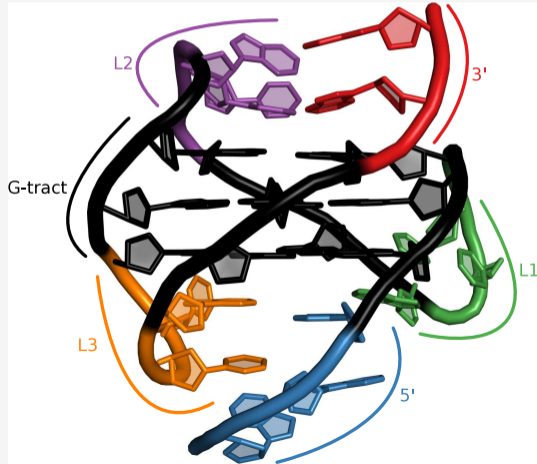- They occur in genomes of different species, including humans

Figure 1: Source: Marsico et al. Whole genome experimental maps of DNA G-quadruplexes in multiple species, NAR 47(8), 2019
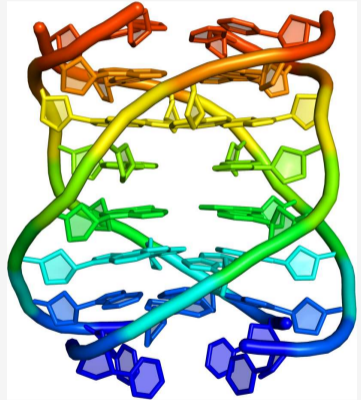
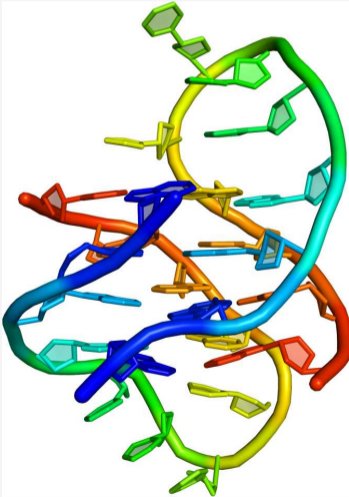# Quadruplex

- Quadruplexes are four-stranded motifs
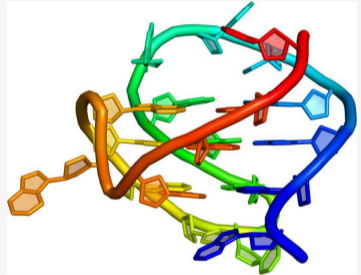- They contain four G-tracts and three loops

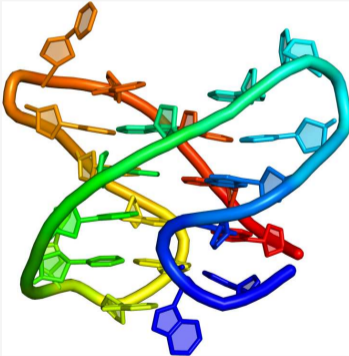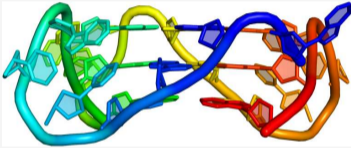# Quadruplex

- Quadruplexes can be unimolecular, bimolecular or tetramolecular

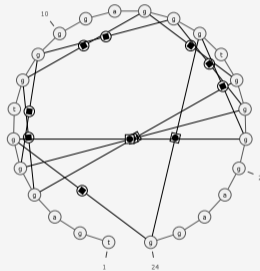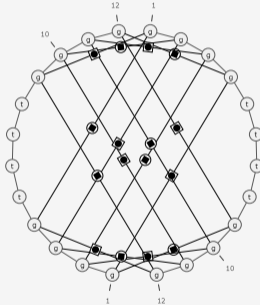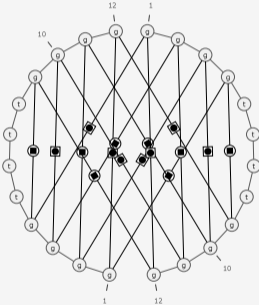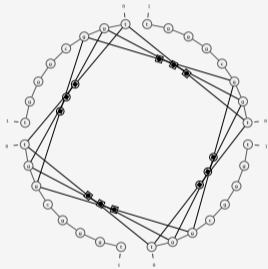# Quadruplex

- Quadruplexes can be parallel, antiparallel or hybrid

VARNA

Two-line dot-bracket

- Nucleotides forming the quadruplex take part in two interactions at once
- This cannot be stored in the dot-bracket format
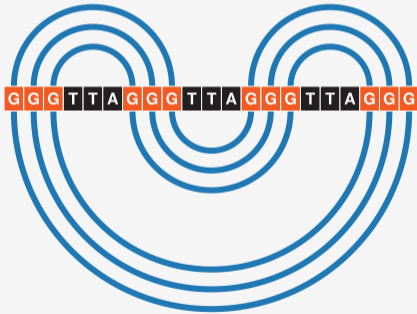- Therefore, we proposed a two-line dot-bracket notation:

```
>antiparallel
GGGTTAGGGTTAGGGTTAGGG
(((...)))...(((...)))
(((...(((...)))...)))
```
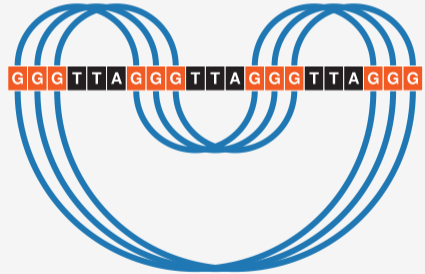
```
>parallel
GGGTTAGGGTTAGGGTTAGGG
([{...)]}...([{...)]}
([{...([{...)]}...)]}
```

R-Chie

- Two-line dot-bracket allows to *abuse* R-Chie to draw both interactions at the same time
- The first line is used to draw the top part
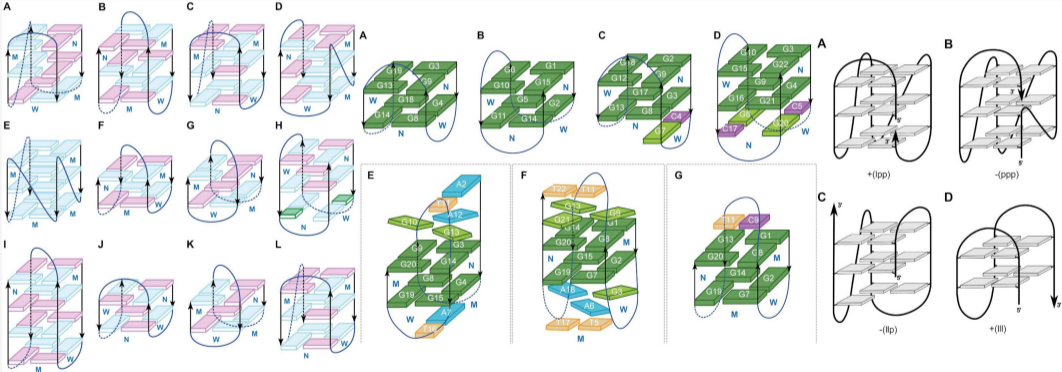- The second line represents the bottom fragment

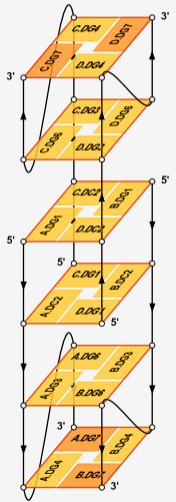antiparallel

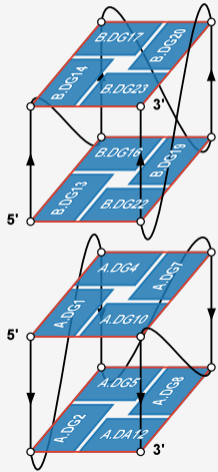parallel

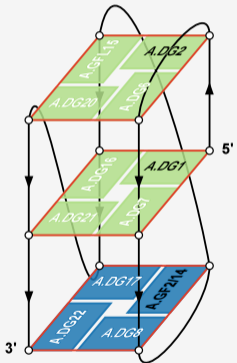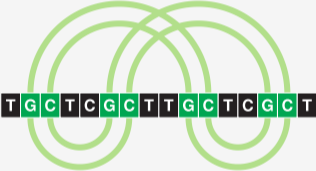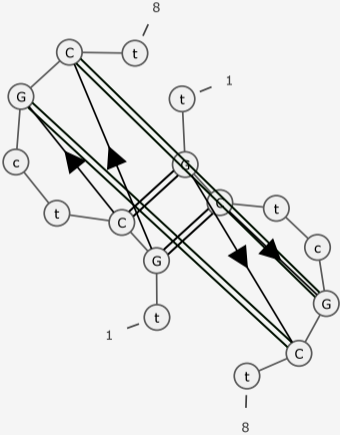# How are quadruplexes usually drawn?

DrawTetrado

- DrawTetrado is a tool to automate quadruplex drawing
- It starts with 3D coordinates and ends with an SVG drawing
- The layout is prepared automatically, with many options to customize:
  - Line widths
  - Colors (*syn / anti*, text, arrows, etc.)
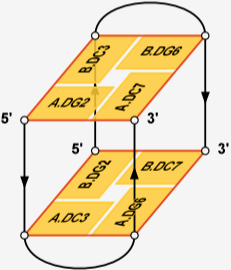 - Fonts
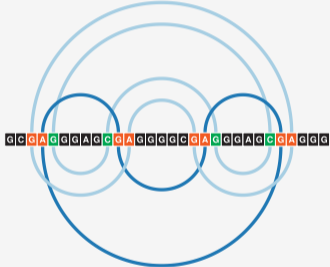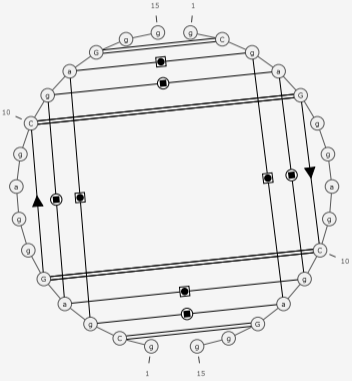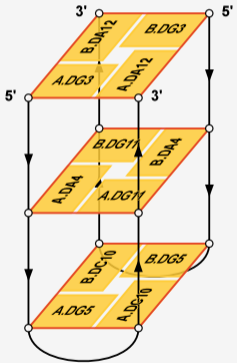 - Spacing / sizing / skew
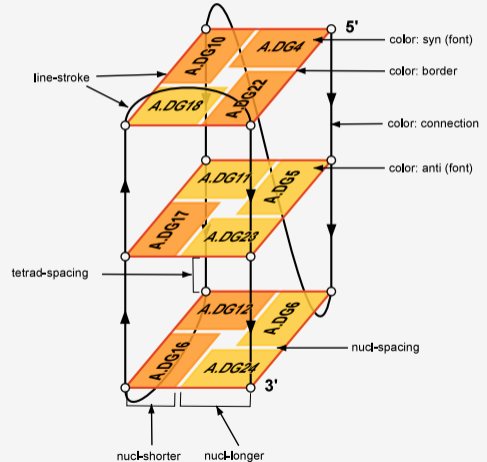
DrawTetrado

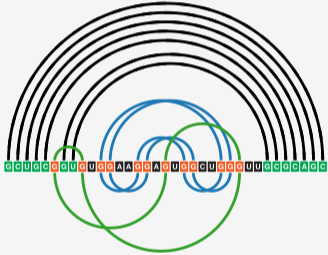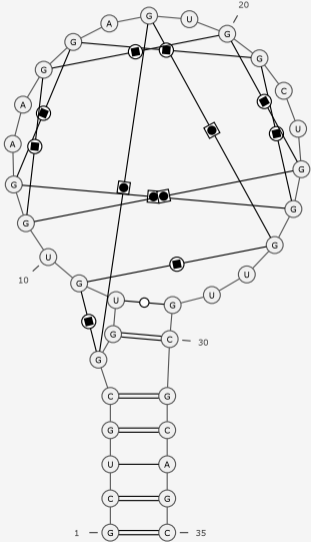# Interesting cases
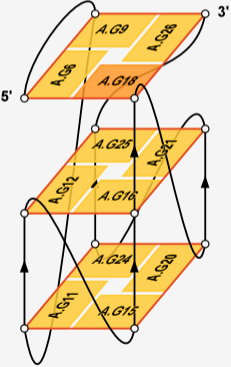

1eu2–h1–q1

Interesting cases

5m1I–h1–q1

Quadruplex & Duplex

5de8-str

Summary

- Quadruplex structures can fold into very diverse and complex 3D shapes

- The 2D structure can be encoded using a two-line dot-bracket notation

- Different visualizations allow to capture different aspects of the motif

- Our quadruplex tools:

  - ElTetrado (https://github.com/tzok/eltetrado)
  - DrawTetrado (https://github.com/michal-zurkowski/drawtetrado)
  - ONQUADRO (https://onquadro.cs.put.poznan.pl)
  - WebTetrado (in progress)