

VARNA: Recent features and alignment related stuffs...

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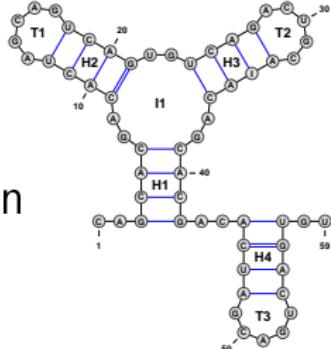
† Université Paris Sud/CNRS/INRIA AMIB – France

* École Polytechnique/CNRS/INRIA AMIB – France

November 14, 2010

Initial goal(s): To draw RNA secondary structure

- ① Webservers companion
- ② Interactive visualization
- ③ Publication-ready drawings production



IRESSite DB summary record describing characteristics of B1001_1_300-301 - Module Testa

File Edit View Hyping Bookmarks Links Help

http://iresite.org/IRESiteDB.php?region=secondary_drawing

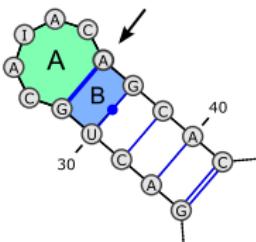
What's this? Label Headers

BRDV1 rRNA within the region 1-28...-10,34 kcal/mol

Remarks:

Genomic probing of B100 secondary structure uses the following buffers:
- priming species B100 (modified composition: 20 mM IRESSiteDB (pH 7.0), 40 mM KCl, 12 mM MgCl₂ for 5 min at 30 °C);
- hybridization buffer B100 (modified composition: 90 mM sodium acetate (pH 5.5), 40 mM KCl, 12 mM MgCl₂, 2.0 mM EGTA).

4.1.1. Enzymes used to characterize at least partially the 2D structure.
4.1.2. Enzyme or a combination of enzymes used in a single experiment with respective buffer:
4.1.3. Experiment with enzyme A:
4.1.4. The temperature (in degrees of Celsius):
4.1.5. Enzyme or a combination of enzymes used in a single experiment with respective buffer:
4.1.6. Conditions:
pH
1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00 8.50 9.00 9.50 10.00
Li⁺ [mM] Na⁺ [mM] K⁺ [mM] Mg²⁺ [mM] Ca²⁺ [mM]
Tris [mM] BSA [mM] HEPES [mM] EGTA [mM] EDTA [mM]

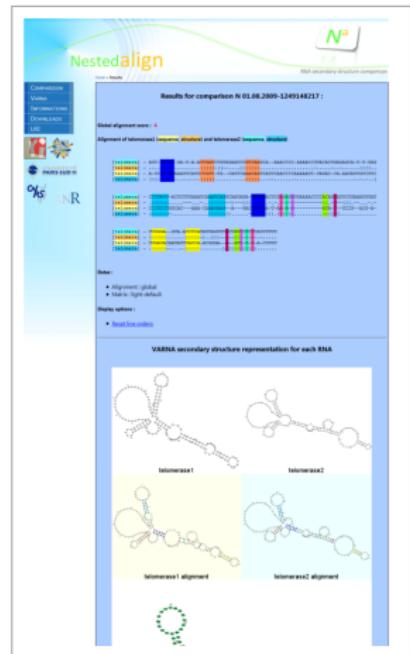


IRESSite DB
<http://iresite.org/>

Varna, Bulgaria

Main features

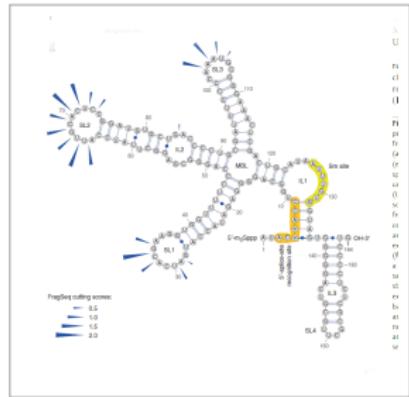
- Client-side
- Cross-platform (Java)
- No external dependencies
- Fully customizable
- Self-adapting to available space
- Accepts most formats (RNAML, CT...)
- Four(+) layout algorithms
- Vector(bitmap output formats
- Standalone editor
- Supports drag and drop
- Command-line version
- Basic support for Pseudonoeuds.
- 3^{ary} interactions ...



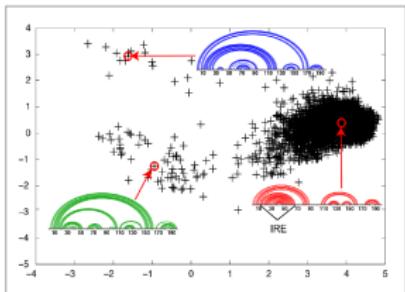
Webserver NestedAlign
<http://nestedalign.lri.fr>

New features

- Session save/restore
→ Snapshots within GUI
 - Better selection mechanisms
 - PseudoBase pseudoknots support
Example: (((...[[[...))])...]))
 - Print structure feature
 - Color maps
 - Bases/Basepairs/regions annotations...
 - Interactive JS library



Underwood et al, Nat. Meth. 2010



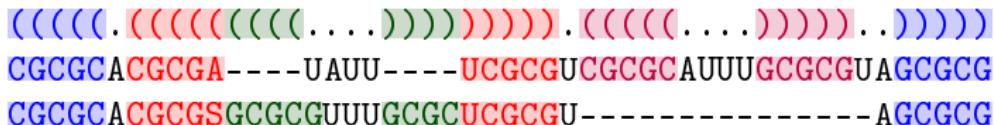
Halvorsen et al. Plos Gen. 2010

▶ Démo site VARNA

Honestly, RNA alignments are mainly about sequences (so far...)

Paradigm: One structure \Rightarrow Many sequences!

Problem: Structural variability leads to horizontal expansion.



But 2^{ary} structure visualization can complement alignments.

Toy example: Two alternative structures:

- Similarities should be self-evident
 - Same annotation/color codes
 - Common parts should be superimposed (easy algorithmically!)
- Differences should *pop up* (Animations can help)
- Alt.: Superstructure (tree alignment à la RNAForester)
- Pattern-based drawing based on coarse-grain layouts (in progress...)

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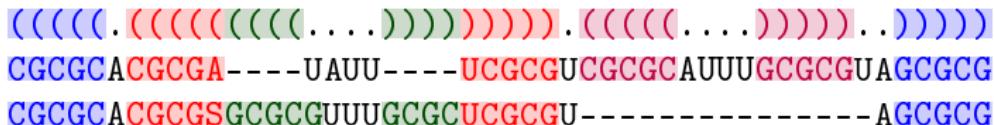
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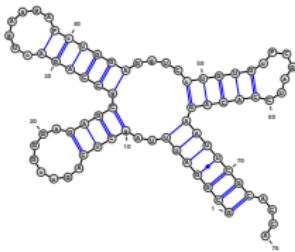
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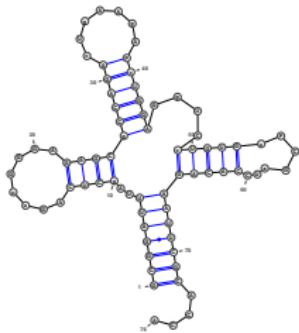
- Pattern-based layouts

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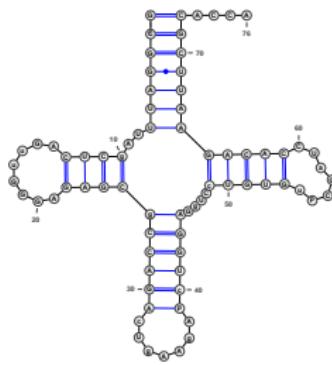
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Radiate algorithm



NAVView algorithm



Standard view

Soon in VARNA...

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For new motifs and families of RNA, automated layouts are ok.

But for *older* classes, people are used to see things in a certain way.

- Draw layout at a coarse-grain level (template)
- Use tree alignment algorithm to map specific RNA sec. str. to template elements (Resilience to structural variations).
- Reconstruct layout based on mapping (technically tricky!)

Bonus: Template discriminated automatically from alignment score.

Dream: A distributed database of templates???

- Automated visualization of multi-strand 3^{ary} motifs

Many thanks to

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VARNA is available at <http://varna.lri.fr>

ROC rocks!

