Übungen zum Sequenzanalyse-Praktikum

Universität Bielefeld, SoSe 2013

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Übungsblatt 13 vom 05.07.2013 Abgabe 10.07.2013

The abstract shape approach abstracts from concrete secondary structures and classifies structures into families that share the same overall structure, respectively shape. The shape representative (*shrep*) of a shape is the structure with the minimum free energy within the family. RNASHAPES implements the concept of abstract shapes defining five different abstraction levels. The abstract shape notation consists of squared brackets '[' and ']' for stacking regions and underscores '_' for unpaired regions.

Exercise 13.1:

Please inspect the consensus secondary structure of the OxyS family taken from Rfam in the figure below. Try to translate the figure into shape strings of level 5, 3 and 1. (Sequence start is at the red helix) For this exercise you need to know the definition of the abstraction levels:



- Level 5 abstracts from all helix interruptions (bulges and internal loops) and ignores single stranded regions. Thus, level 5 accounts only for hairpins and multiloops. The level 5 shape of a tRNA clover leaf, which consists of three adjacent hairpins that are nested in one multiloop, would be [[][]].
- In addition to level 5, **level 3** displays every helix interruption by an extra pair of nested, squared brackets. E.g. a hairpin with one bulge to the left would result in [[]].
- Level 1 additionally accounts for each unpaired region, except the innermost loop of a hairpin. The hairpin with one bulge to the left would end up as [_[]].

Level	Shape string for <i>OxyS</i>
5	
3	
1	1

Exercise 13.2:

The biological active structure sometimes hides in the "near" suboptimal search space. But what is "near" and how many predictions must be inspected by eye? With an suboptimal energy range of 5 kcal/mol, RNASUBOPT provides 309 structures for the alanine tRNA sequence of *Natronobacterium pharaonis*. Increasing the energy range to 10 kcal/mol result in 19,322 structures. Scanning through the result list, ordered by energy, reveals the first cloverleaf structure at rank 123!

Can we get an easier overview of the search space? Perform shape foldings of the alanine tRNA sequence of *Natronobacterium pharaonis* and complete table 2. Re-run your query with different settings for the "sub-optimal energy deviation" (h) and the "shape level" (i).

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- 1. Browse to http://bibiserv.techfak.uni-bielefeld.de/rnashapes, follow the link to "the latest version of RNASHAPES" and go to the Submission tab (a).
- 2. Select the "shapes" function of RNASHAPES (b).
- 3. Click on the "example" (d) button to get the alanine tRNA sequence.
- 4. Use default settings (f) in the next dialog and finally "start calculation" (g).

Level	# of alternative shapes for kcal/mol		rank of shapes fo	cloverleaf or kcal/mol	Structure / shape
	5	10	5	10	
5					
3					
1					
0	309	19,322	123	123	((((((())))))))))))))))))))))))))))

Exercise 13.3:

What is common to all abstraction levels? What do they abstract from?

Exercise 13.4:

Look at the results for the alanine tRNA sequence. Compare the structures with shape [[][]] for level 5 and 3. Are they equivalent? Why (not)?