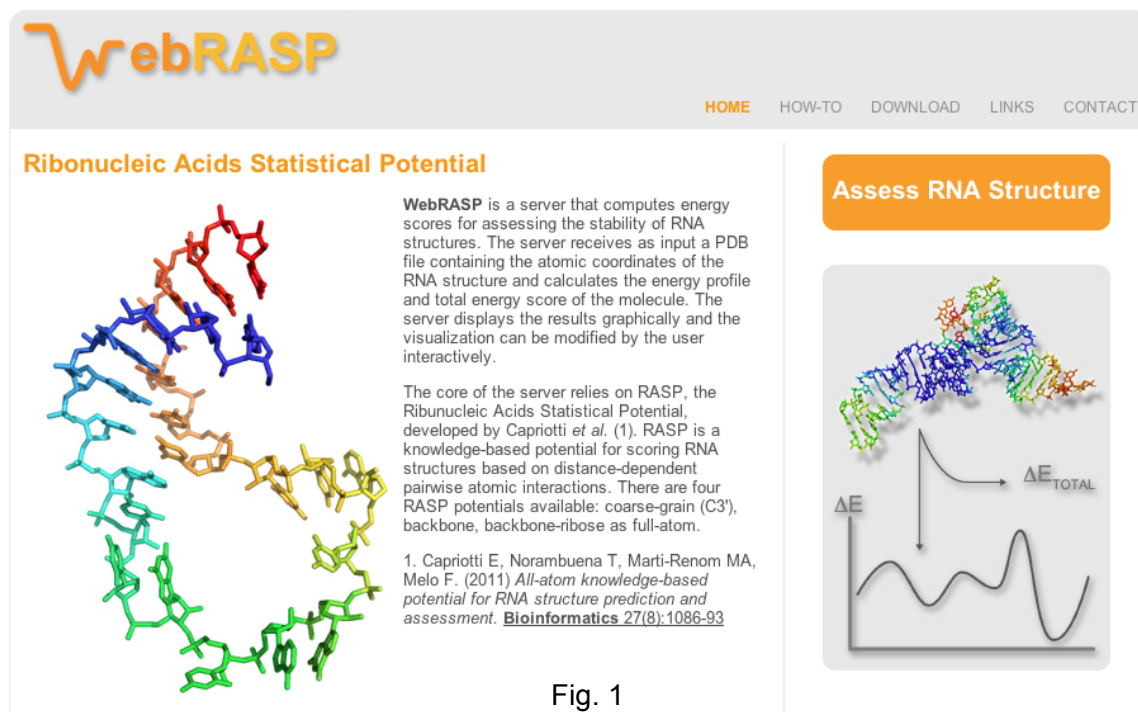


Tutorial

WebRASP is the web server implementation of the Ribonucleic Acid Statistical Potential (RASP). The RASP program can be also run locally by downloading it from the web page <http://melolab.org/webrasp/download.php>. The web is accessible from the home page of WebRASP clicking the button *Assess RNA Structure* (see Fig. 1). WebRASP evaluates the total energy and the energy profile of a given RNA structure. The RNA structure can be scored following the next steps.



WebRASP

HOME HOW-TO DOWNLOAD LINKS CONTACT

Ribonucleic Acids Statistical Potential

WebRASP is a server that computes energy scores for assessing the stability of RNA structures. The server receives as input a PDB file containing the atomic coordinates of the RNA structure and calculates the energy profile and total energy score of the molecule. The server displays the results graphically and the visualization can be modified by the user interactively.

The core of the server relies on RASP, the Ribonucleic Acids Statistical Potential, developed by Capriotti *et al.* (1). RASP is a knowledge-based potential for scoring RNA structures based on distance-dependent pairwise atomic interactions. There are four RASP potentials available: coarse-grain (C3'), backbone, backbone-ribose as full-atom.

1. Capriotti E, Norambuena T, Marti-Renom MA, Melo F. (2011) *All-atom knowledge-based potential for RNA structure prediction and assessment*. [Bioinformatics](#) 27(8):1086-93

Assess RNA Structure

ΔE ΔE_{TOTAL}

Fig. 1

Step 1

In the first page the user need to upload the file in PDB format of the RNA structure.

Step 2

When the RNA structure is provided, in the next page the server allows to select the following options: i) PDB chain; ii) potential type (C3', Backbone, Backbone+Ribose, All atoms); iii) the size of the sliding window used to smooth the energy profile (see Fig. 2). After selecting the options, by clicking the button *SUBMIT*, the server starts the evaluation of the RNA structure.

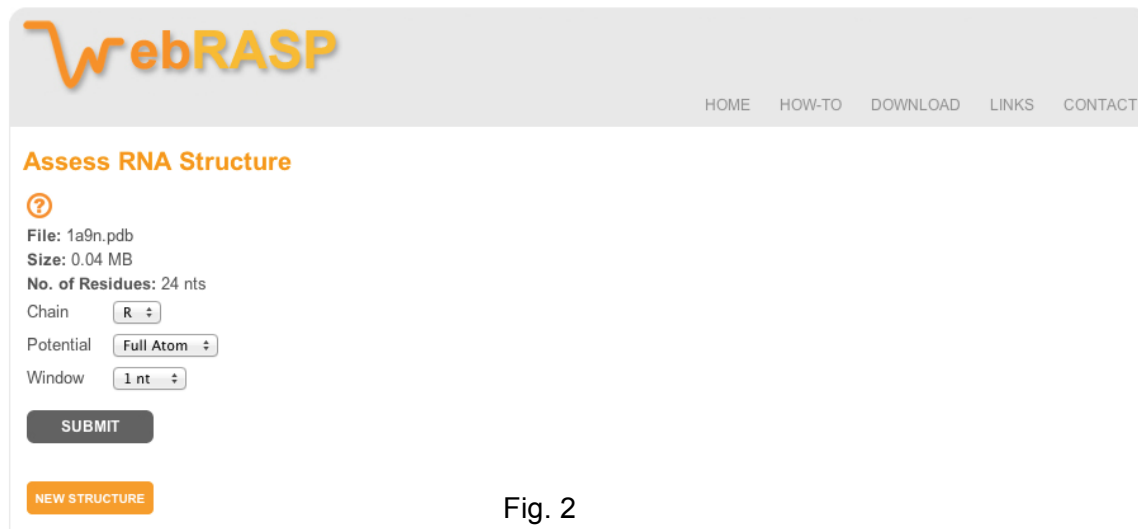


Fig. 2

Step 3

In the last page the server presents the output of the WebRASP server (Fig 3). In the right side of the page the values of the *Energy Score*, the *Number of Contacts* and the *Normalized Energy* are reported. In the center of the output page, the server shows the RNA structure using the JMol applet and coloring the nucleotides according to their energy in the profile. In the bottom, the plot of the energy profile is shown. The energy values corresponding to each nucleotide can be downloaded clicking on the *Profile* link on the *Download Data* section of the output page or displayed on the JMol applet moving the mouse over the energy profile plot. The section Visualization Controls allows to change the color of the nucleotides in the structure according to their energy values.

The options used in the calculation of the energy profile can be modified in the left side of the output web page. The method can be used to evaluate the effect of single point mutations calculating the energy change between the wild-type RNA structure and those obtained after mutation. Example of this task are provided in the RASP paper (Capriotti et al. Bioinformatics 2011).

Assess RNA Structure



File: 1a9n.pdb
 Size: 0.04 MB
 No. of Residues: 24 nts
 Chain:
 Potential:
 Window:

SUBMIT

NEW STRUCTURE



Structure score

Energy score: -9,869.61 kcal/mol
 Number of contacts: 66,447 contacts
 Normalized energy: -0.1485 kcal/mol/cont

Download data

Profile:

Visualization controls

	Value	Custom	Color
Max:	-54.39	<input type="text" value="-54.39"/>	<input type="text" value="#FF0000"/>
Mid:	-878.40	<input type="text" value="-878.40"/>	<input type="text" value="#FFFFFF"/>
Min:	-1702.41	<input type="text" value="-1702.41"/>	<input type="text" value="#0000FF"/>
<input type="checkbox"/> Show residue labels			<input type="text" value="#FFFF00"/>

UPDATE DEFAULT

Energy/Score profile for Chain R

Color for highlighting residues:

Drag the profile

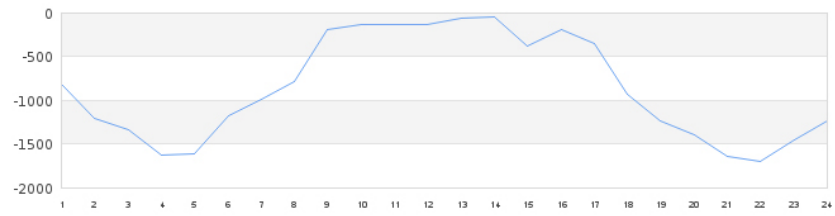


Fig. 3