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Regular paper

New functionality of the RNAComposer: an application to shape the axis of miR160 precursor structure

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RNAComposer is a fully automated, web-interfaced system for RNA 3D structure prediction, freely available at http://rnacomposer.cs.put.poznan.pl/ and http://rnacomposer.ibch.poznan.pl/. Its main components are: manually curated database of RNA 3D structure elements, highly efficient computational engine and user-friendly web application. In this paper, we demonstrate how the latest additions to the system allow the user to significantly affect the process of 3D model composition on several computational levels. Although in general our method is based on the knowledge of secondary structure topology, currently the RNAComposer offers a choice of six incorporated programs for secondary structure prediction. It also allows to apply a conditional search in the database of 3D structure elements and introduce user-provided elements into the final 3D model. This new functionality contributes to a significant improvement of the predicted 3D model reliability and it facilitates a better model adjustment to the experimental data. This is exemplified based on the RNAComposer application for modelling of the 3D structures of precursors of the miR160 family members.

Key words: RNA 3D structure prediction, RNAComposer, plant miRNA precursor

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Abbreviations:

Table S1. Structural elements selected for miR160 precursors' modeling in the batch (with new functions) and the interactive mode.

miR160a

Secondary structure element			RNA FRABASE search pattern	3D element introduced by the user in batch mode					3D element used by RNAComposer in interactive mode				
Id	Topology	Description		PDB id chain	Position	Topology	Res. [Å]	PSI [%]	PDB id chain	Position	Topology	Res. [Å]	PSI [%]
L1	CCU (.(AUG).)	mismatch	NCN (.(NUN).)	1VQ8 0	763-765, 899-901	CCG (.(CUG).)	2.20	66.66	3V2F AB	586-588, 597-599	CCU (.(AUG).)	2.70	100.00
L2	CCU (.(GAG).)	mismatch	NCN (.(NAN).)	4FE5 B	25-27, 43-45	UCG (.(CAA).)	1.32	33.33	1KFO AB	6-8, 30-32	CCU (.(GAG).)	1.60	100.00
L3	UAU (.(GGA).)	mismatch	NAN (.(NGN).)	157D AB	8-10, 15-17	UAG (.(CGA).)	1.80	66.66	3U5D BA	1039-1041, 1009-1011	UAU (.(AGA).)	3.00	83.33
L4	CUG (.(CCG).)	mismatch	NUN (.(NCN).)	1YHQ 0	558-560, 597-599	CUU (.(ACG).)	2.40	66.66	1VQ8 0	898-900, 762-764	CUG (.(CCG).)	2.20	100.00
L5	GCCC (..(GACC)..)	tandem mismatches	NYYN (..(NRYN)..)	3WBM XY	10-13, 14-17	ACCC (..(GACU)..)	2.00	75.00	1JID B	4-7, 22-25	GACC (..(GACC)..)	1.80	87.50

miR160b

Secondary structure element			RNA FRABASE search pattern	3D element introduced by the user in batch mode					3D element used by RNAComposer in interactive mode				
Id	Topology	Description		PDB id chain	Position	Topology	Res. [Å]	PSI [%]	PDB id chain	Position	Topology	Res. [Å]	PSI [%]
L1	CCU (.(AAG).)	mismatch	NCN (.(NAN).)	4FE5 B	25-27, 43-45	UCG (.(CAA).)	1.32	33.33	3U5H BA	2338-2340, 1895-1897	CCU (.(AAG).)	3.00	100.00
L2	UCCC (..(GAGUA)...)	asymmetrical internal loop	(..( )...)	2OE5 AB	1407-1410, 1490-1494	CGCU (..(AAAAG)...)	1.51	22.22	2KRL AB	72-75, 80-84	UCCC (..(GGGUG)...)	-[1]	77.78
L3	CAA (.(UAG).)	mismatch	NAN (.(NAN).)	4J50 AB	7-19, 13-15	CAG (.(CAG).)	1.65	66.66	1VQO 0	2359-2361, 2423-2425	CAA (.(UAG).)	2.20	100.00
L4	GAAAACA (.....(UCAC)..)	asymmetrical internal loop	(.....( )..)	4KZD R	19-25, 63-66	GAAGGAC (.....(GAGC)..)	2.19	36.36	1P9X AB	1668-1674, 1986-1989	GAGAACC (.....(GGAC)..)	3.40	63.64

miR160c

Secondary structure element			RNA FRABASE search pattern	3D element introduced by the user in batch mode					3D element used by RNAComposer in interactive mode				
Id	Topology	Description		PDB id chain	Position	Topology	Res. [Å]	PSI [%]	PDB id chain	Position	Topology	Res. [Å]	PSI [%]
L1	CCU (.(AAG).)	mismatch	NCN (.(NAN).)	4FE5 B	25-27, 43-45	UCG (.(CAA).)	1.32	33.33	3U5H BA	2338-2340, 1895-1897	CCU (.(AAG).)	3.00	100.00
L2	CCU (.(AAG).)	mismatch	NCN (.(NAN).)	4FE5 B	25-27, 43-45	UCG (.(CAA).)	1.32	33.33	3U5H BA	2338-2340, 1895-1897	CCU (.(AAG).)	3.00	100.00
L3	CGAG (..(CCGG)..)	tandem mismatches	NRRN (..(NYRN)..)	2ZJR X	1491-1494, 1530-1533	CAAG (..(UCAG)..)	2.91	50.00	3J3F AB	490-493, 574-577	CGUG (..(CCGG)..)	5.00	87.50
L4	GAUAC (...(GC))	asymmetrical internal loop	(...( ))	397D AB	22-26, 39-40	AUCUG (...(CU))	1.30	0.00	1U3K BA	29-33, 6-7	GAUAU (...(AC))	-[1]	71.43

[1] the corresponding RNA structure was determined by NMR spectroscopy

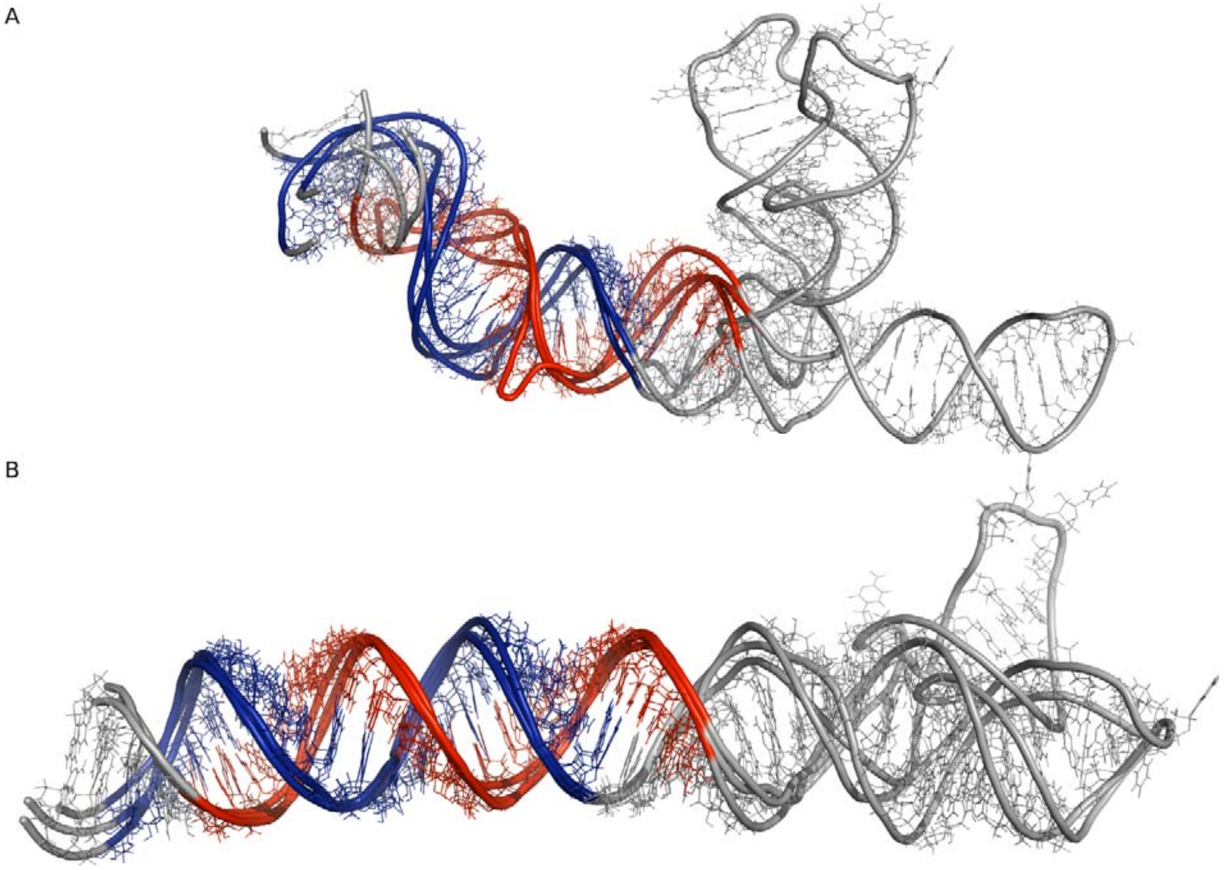

Figure S1. Superimposed 3D models of miR160a, miR160b and miR160c precursors predicted with the RNAComposer interactive (A) and batch mode with new functionality (B). Superposition is based on miRNA (red). miRNAs* are drawn in blue.

PDB files availability

PDB files with 3D models of miR160 precursors predicted by RNAComposer with new functionality and the reference structure are available for download at http://www.cs.put.poznan.pl/mantczak/abp-antczak-suppl.zip