



User Guide

Version 1.1

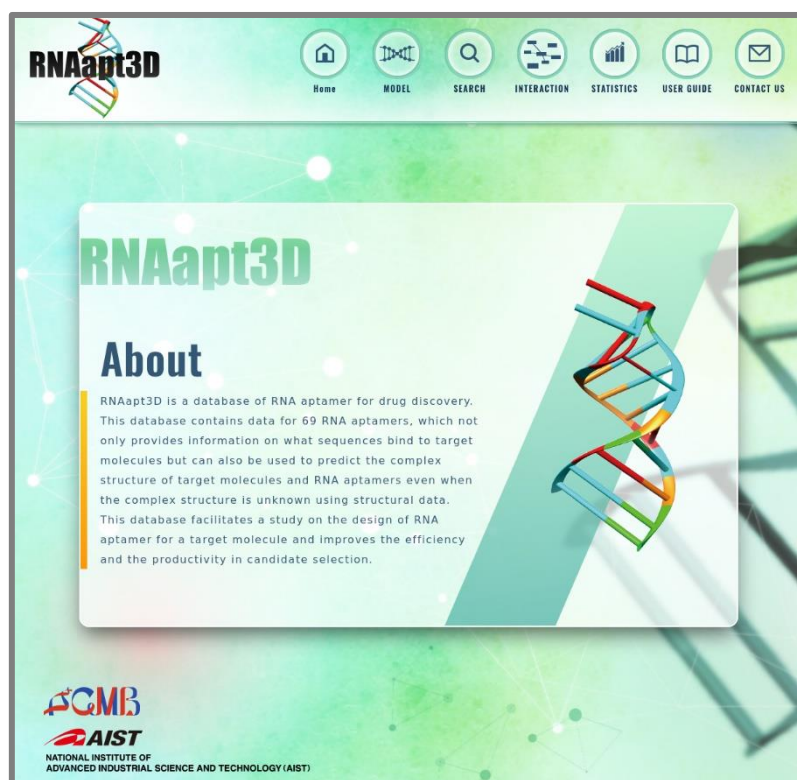
2022/4/27

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1 Introduction

RNAapt3D is RNA aptamer database to support the development of new RNA aptamer. This database contains data for 69 RNA aptamers and provides the RNA sequence, sequence length, target molecule, adaptation diseases, product name, clinical phase, remark, structure string, secondary structure, and tertiary structure. RNAapt3D lets you creatively promote on your project for the development of new RNA aptamer.



2 Querying the Database

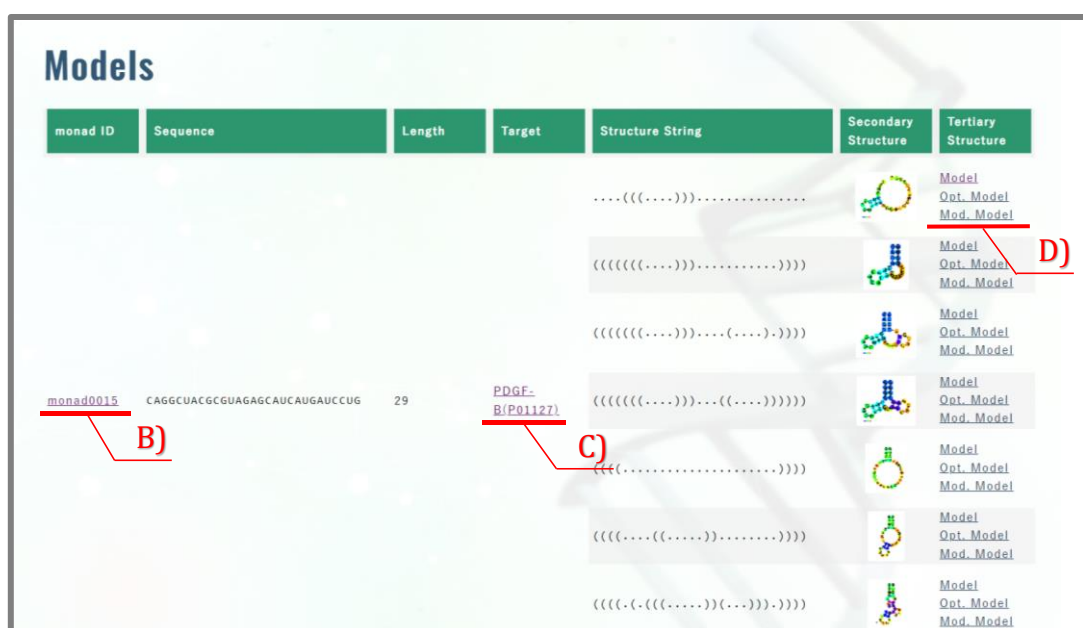
2.1 Search of information of Model








Menu items are shown at the top of RNAapt3D page.



A) Browser aptamer models

Click on the “Model” at the top menu, you can browser the RNA sequence, the target protein, and the structural information of each entry (monad’s ID).



monad ID	Sequence	Length	Target	Structure String	Secondary Structure	Tertiary Structure
			(((.....)).....		Model Opt_Model Mod_Model
				(((((((.....)).....)))		Model Opt_Model Mod_Model
				(((((((.....))....(.....))		Model Opt_Model Mod_Model
<u>monad0015</u>	CAGGCUACGCGUAGAGCAUCAUGAUCCUG	29	<u>PDGF-B(P01127)</u>	(((((((.....))....(.....))		Model Opt_Model Mod_Model
				(((.....)).....		Model Opt_Model Mod_Model
				(((.....(((.....)).....)))		Model Opt_Model Mod_Model
				(((.....(((.....)).....))		Model Opt_Model Mod_Model

B) View detail information of RNA aptamer

Click on the “monad’s ID” (for example: monad0015) in the list, the detail of its RNA aptamer will be shown.

Detail of monad0015

Aptamer Detail

monad ID	Length	Target Molecule	Remark
monad0015	29	PDGF-B (P01127)	Fovista is a new drug expected as a remedy for neovascular age-related macular degeneration. Currently, 3 kinds of tests shown below has been initiated. - a phase Ib randomized, double-masked, controlled trial to establish the safety and efficacy of intravitreal administration of Fovista administered in combination with Avastin compared to Avastin monotherapy in subjects with subfoveal neovascular age-related macular degeneration. - a phase III randomized, double-masked, controlled trial to establish the safety and efficacy of intravitreal administration of Fovista (Anti PDGF-B pegylated aptamer) administered in combination with either Avastin or Eylea compared to Avastin or Eylea monotherapy in subjects with subfoveal neovascular age-related macular degeneration - a phase III randomized, double-masked, controlled trial in order to establish the safety and effectiveness of intravitreal administration with combination of Fovista and Lucentis compared with administration of only Lucentis

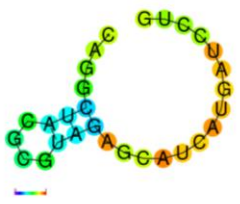
Sequence
CAGGCUACGCGUAGAGCAUCAUGAUCCUG

Adaptation Disease
subfoveal neovascular age-related macular degeneration

Product Name
Fovista

Phase
III

Structure monad0015-1

Parameter	Secondary Structure
CentroidFold: CONTRAFold 2*1	
Structure String ...((.....)).....	
Flip Position *.....	
Tertiary Structure Rascal Model Optimized Model Modified Model	

[Download](#)

Tertiary structure model PDB file can be downloaded by clicking icons beside model links.

C) Inspect target protein

Click on the “Target protein’s name” (for example: PDGF-B) in the list, then Uniprot page related to its protein will open in new window. Confirm the detail of its protein.

The screenshot shows the UniProtKB entry for Platelet-derived growth factor subunit B (P01127). The page is organized into several sections:

- Entry:** Protein: Platelet-derived growth factor subunit B; Gene: PDGFB; Organism: Homo sapiens (Human); Status: Reviewed - Annotation score: 5 - Experimental evidence at protein level¹.
- Function:** Growth factor that plays an essential role in the regulation of embryonic development, cell proliferation, cell migration, survival and chemotaxis. Potent mitogen for cells of mesenchymal origin (PubMed:26599395). Required for normal proliferation and recruitment of pericytes and vascular smooth muscle cells in the central nervous system, skin, lung, heart and placenta. Required for normal blood vessel development, and for normal development of kidney glomeruli. Plays an important role in wound healing. Signaling is modulated by the formation of heterodimers with PDGFA (By similarity).
- Sites:** A table listing two sites involved in receptor binding.
- GO - Molecular function:** chemoattractant activity, collagen binding, growth factor activity.

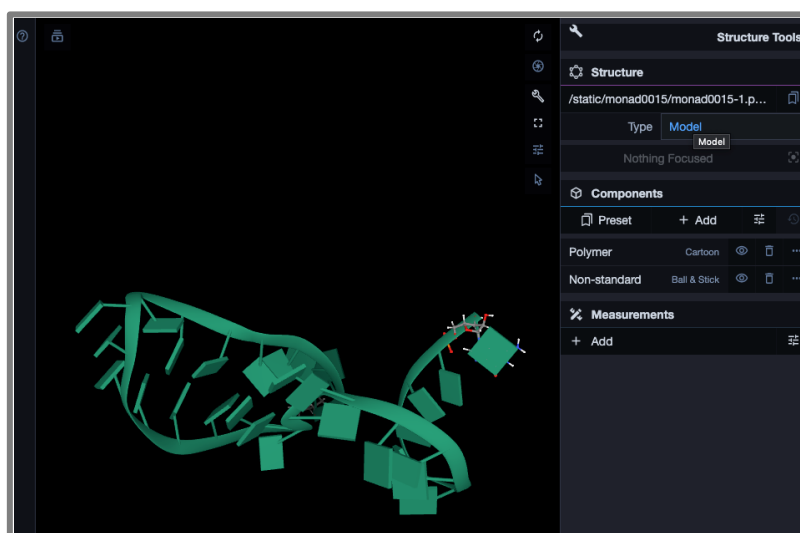
Feature key	Position(s)	Description	Actions	Graphical view	Length
Site ¹	108	Involved in receptor binding			1
Site ¹	111	Involved in receptor binding			1

D) View tertiary structure

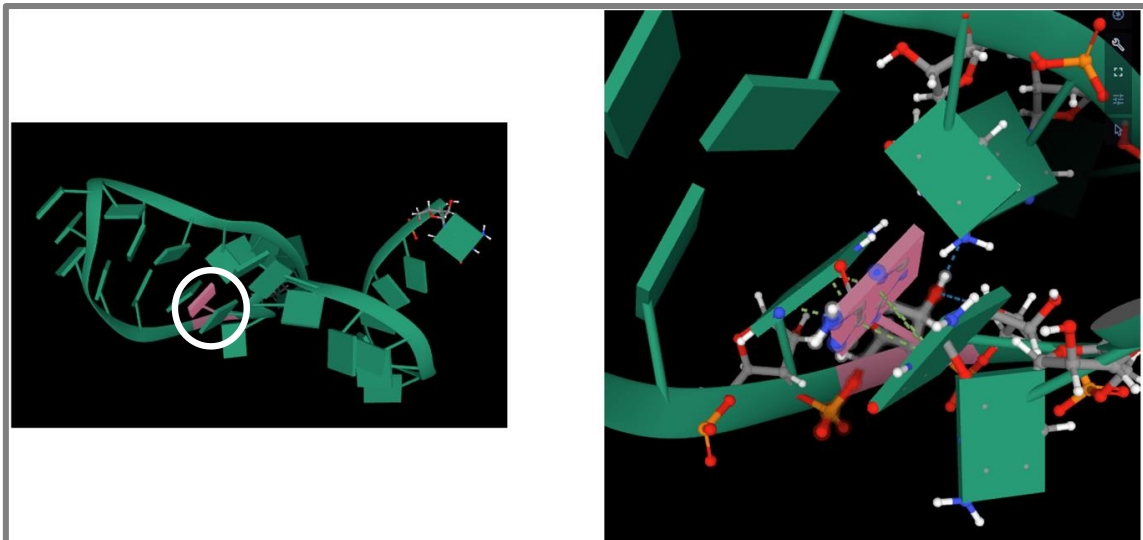
Click on the “Model”, “Opt. Model”, or “Mod. Model” at the right tertiary structure section. PDBe Mol* Viewer page will open in new window.

“Model” structure was predicted by Rascal. “Opt. Model” and “Mod. Model” structures were relaxed by MD simulations for Rascal model structure. MD simulations from 5 to 10 ns were classified into 10 clusters according to their structural similarities using a k-means method. Ten representative structures for each cluster are stored as the optimized model.

The tertiary structure can be directly confirmed.

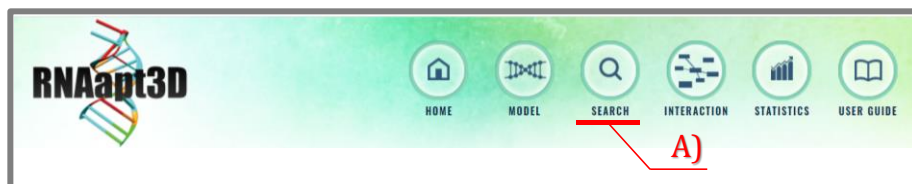


Click on the specific nucleotide on this viewer. Some interactions between its nucleotide and other nucleotides can be confirmed.



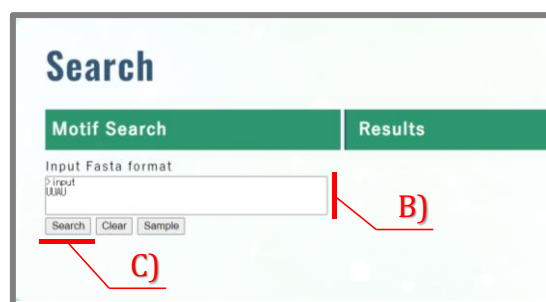
2.2 Search for RNA motif

You can search RNA sequence in RNAapt3D database.



A) Navigate to search page

Click on the “Search” at the top.



B) Enter the RNA sequence

Enter the RNA sequence in Motif Search, where the input sequence can be in upper or lower case. If you click “Sample” button, an example sequence will be entered.

C) Execute Search

Click on the “Search” button, Motif search will take a few tens of seconds.

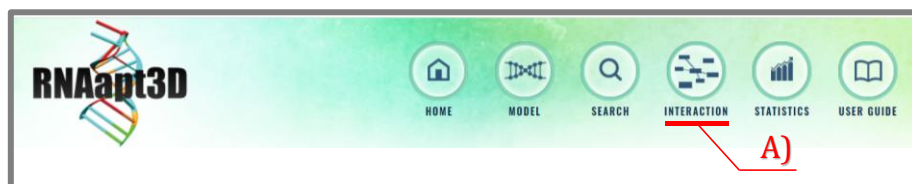
Some entries containing a given RNA sequence and the predicted base flip positions for these entries will be displayed.

Search

Motif Search	Results
Input Fasta format UUU Search Clear Sample	> monad0024 CGGAAUCAGUGAAUGCUUAUACAUCG -----UUAU----- ***** (24-1) **** (24-2) *** (24-3) ***** (24-4) ***** (24-5)
	> monad0049 AAUGAGUGGUUAUUCGUU -----UUAU----- * (49-1) ----- (49-2) *** (49-3) * (49-4)
	> monad1011 UUGCUGGAAUGCGUUAUAGUCUCUUAGGUGUGUA -----UUAU----- ***** (1011-1)

3 Interaction

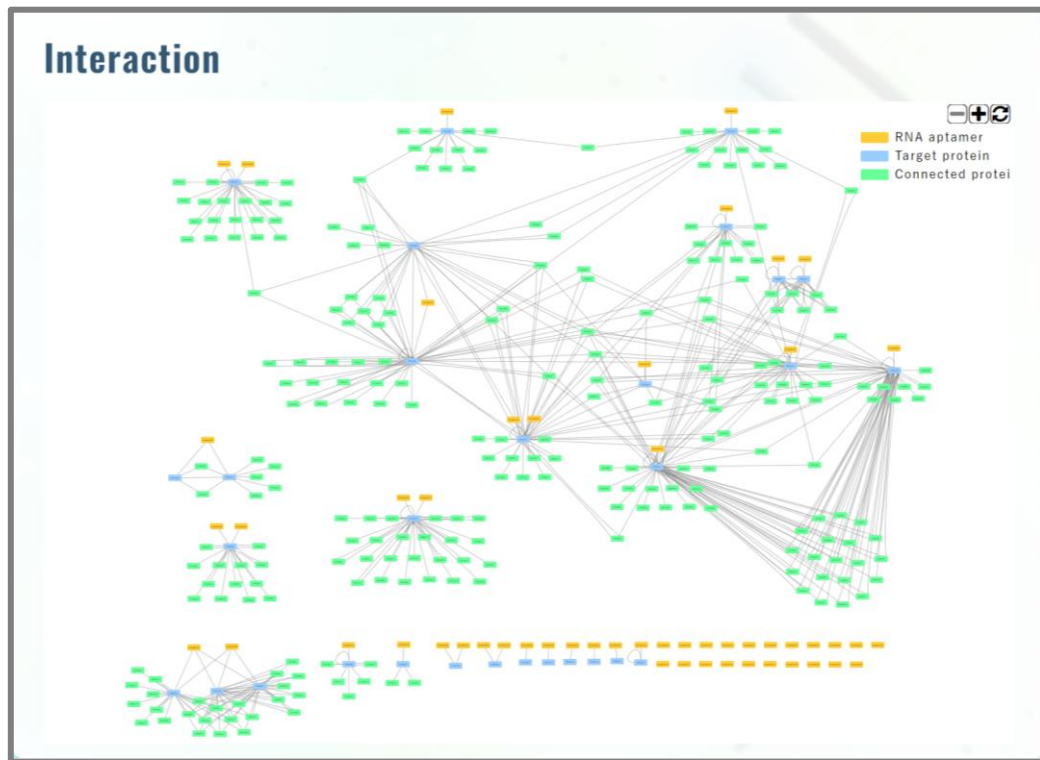
You can check interactions between aptamer and protein, and between protein and protein.



A) Move to interaction page

Click on the “Interaction” at the top menu.

It shows RNA aptamer (orange square)-Target proteins (blue square) interactions. The proteins (green square) connected to the target proteins (blue square) are obtained by projecting on protein-protein interaction network of Human Protein Reference Database.



The + and- signs in the upper right zoom in and out of the network diagram.

4 Statistics

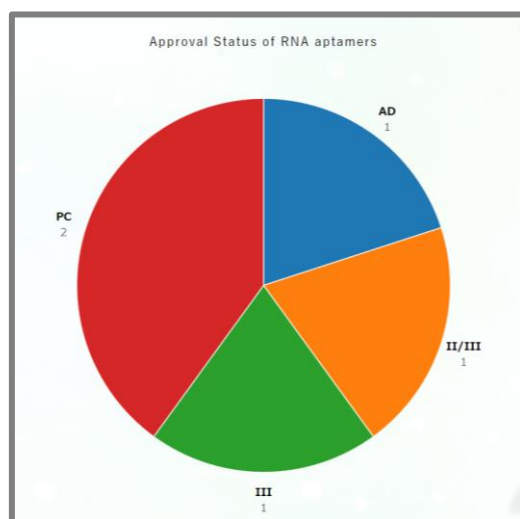
Statistical information is on Statistics page.



A) Move to statistics page

Click on the “Statistics” at the top.

The number of RNA aptamer included this database for each clinical phase can be confirmed.



The number of RNA aptamer included this database for each target protein can be confirmed.

Target Protein	Number of RNA aptamers
AXL	1
C5	2
CCL2	1
CGA	1
CXCL8	1
EGFR	1
EIF4A1	2
EPCAM	1
ERBB2	1
FGF2	1
GRK2	2
IL6	2
IL6R	1
ITGAV	1
LOC8261245	1
MDK	1

5 Contact Us

RNAapt3D

URL: <https://rnaapt3d.medals.jp>



If you have any questions or comments, please contact the following e-mail address.

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