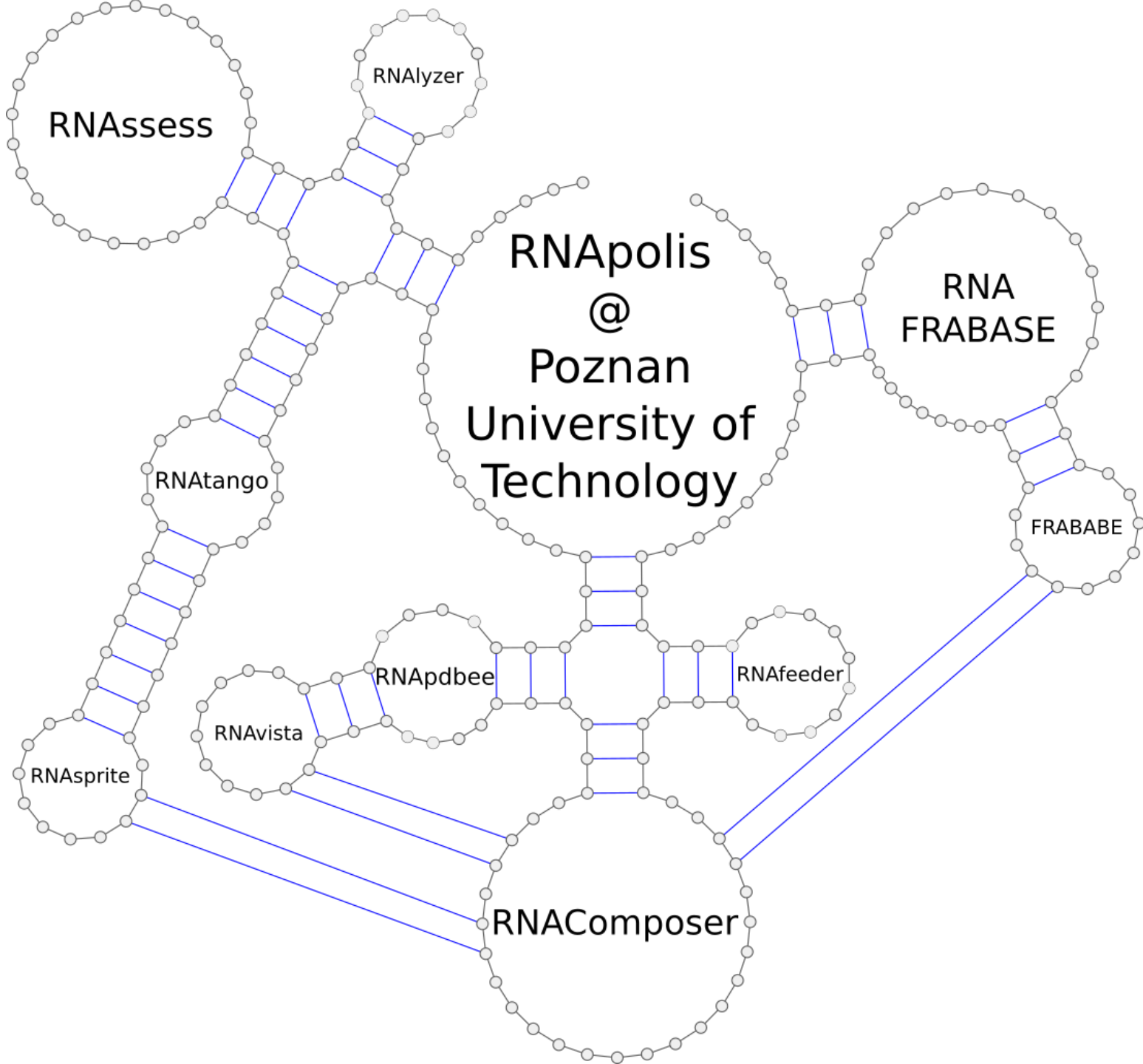


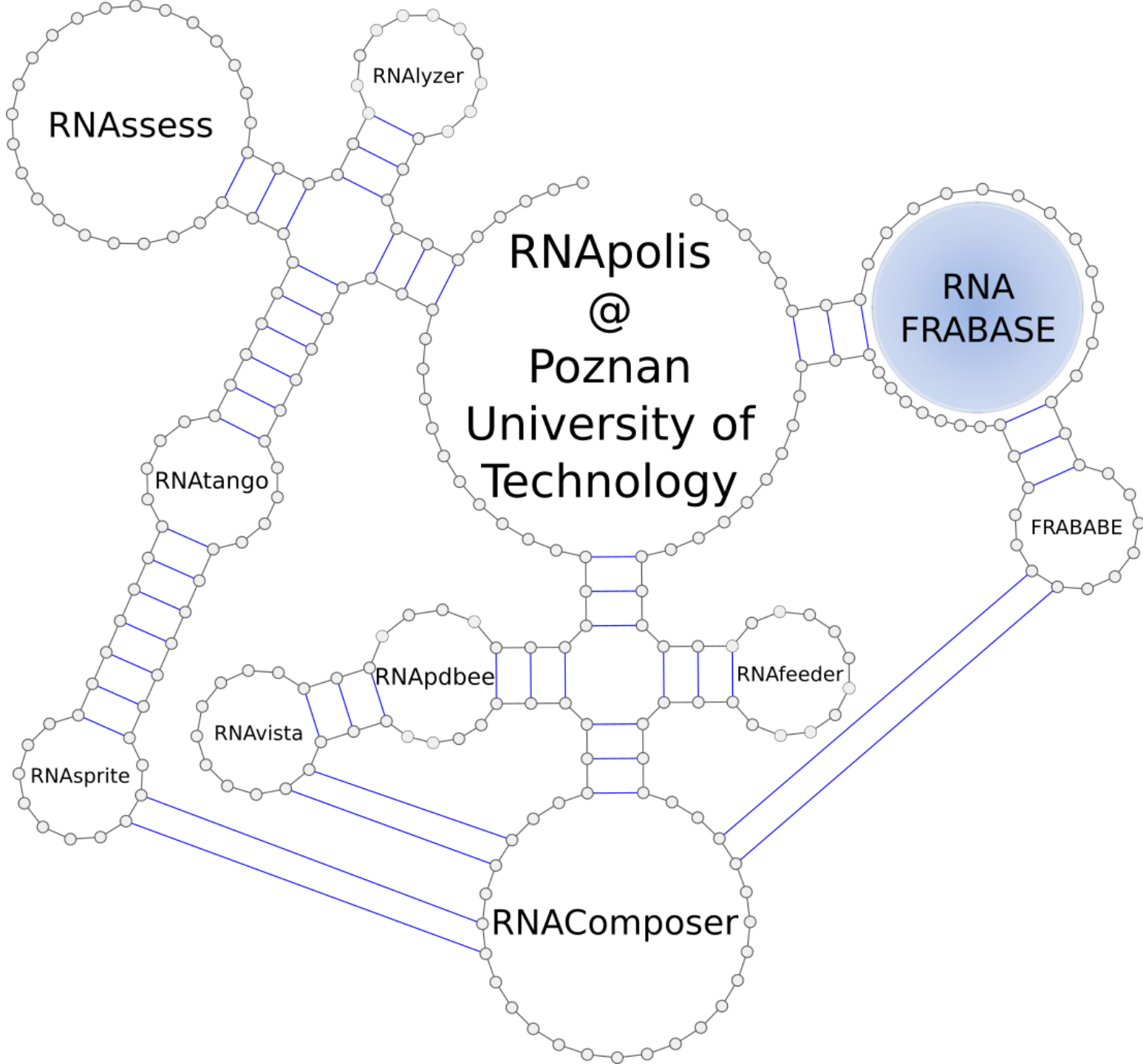
# RNApolis for RNA structure analysis



Marta Szachniuk

Poznan University of Technology  
& Institute of Bioorganic Chemistry, Polish Academy of Sciences

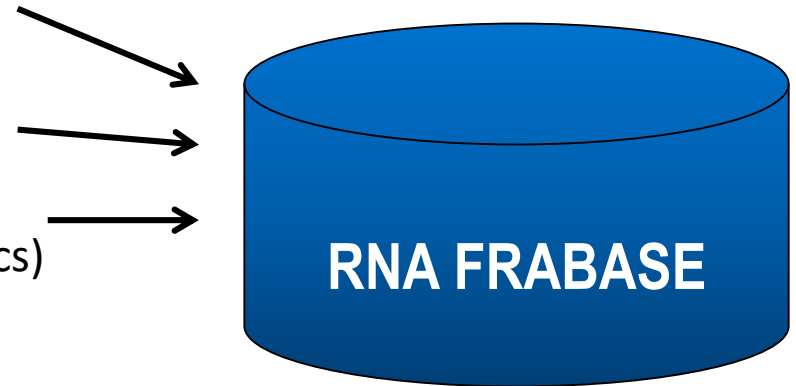




# RNA FRABASE: RNA fragments database & search engine

## Collects structural data & models relationships between them

- sequences
- atom coordinates
- torsional & pseudotorsional angles
- sugar-pucker parameter
- base pair classification
- base-base & inter base pair parameters
- secondary structure (dot-bracket, graphics)



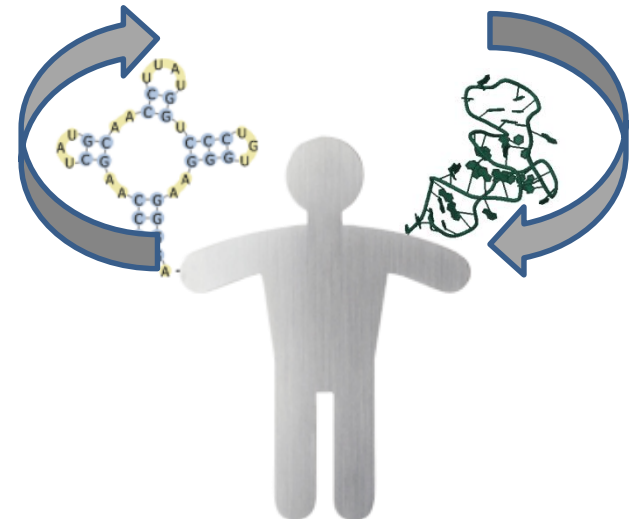
## Allows for easy/fast search for 3D fragments

Input (query):

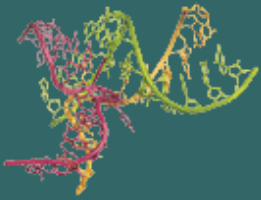
- Sequence and / or
- Secondary structure (dot-bracket)

Output:

List of PDB ids + structure parameters



http://rnafrabase.cs.put.poznan.pl/



# RNA FRABASE 2.0

## RNA FRAGments search engine & dataBASE

### Search

Structural elements

Secondary structures

Help

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References

Links

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You are 2233855 visitor.  
Currently 1 users online.

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Laboratory of Structural  
Chemistry of Nucleic Acids &  
Laboratory of Bioinformatics,  
Institute of Bioorganic  
Chemistry,  
Polish Academy of Sciences

**RNA FRABASE:** an engine with database to search the three-dimensional fragments within 3D RNA structures using as an input the sequence(s) and / or secondary structure(s) given in the dot-bracket notation.

Database in its 2.0 version contains (updated 2013-11-08):

- RNA sequences and secondary structures, described in dot-bracket notation, derived from the 2369 PDB-deposited RNA structures and their complexes,
- atom coordinates of the unmodified and modified nucleotide and nucleoside residues (1677541 cases) copied out from the PDB-deposited RNA structures,
- torsion and pseudotorsion angle values, sugar pucker parameters and complete classification of base pair types given for the PDB-deposited RNA structures.

Sequence(s) and / or secondary structure(s):

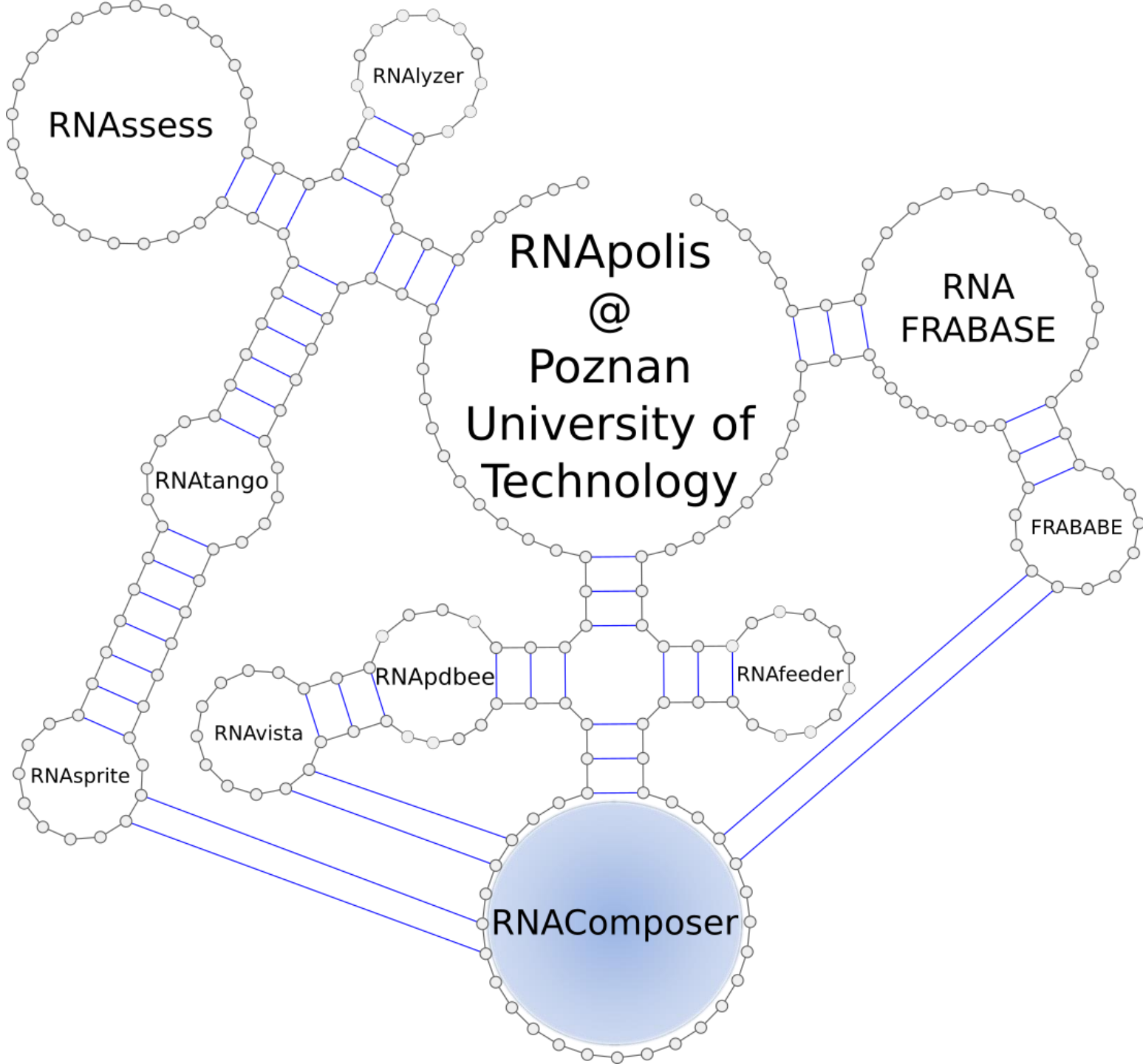
Load example: [1](#) [2](#) [3](#) [4](#) [5](#) [6](#)

No file selected.

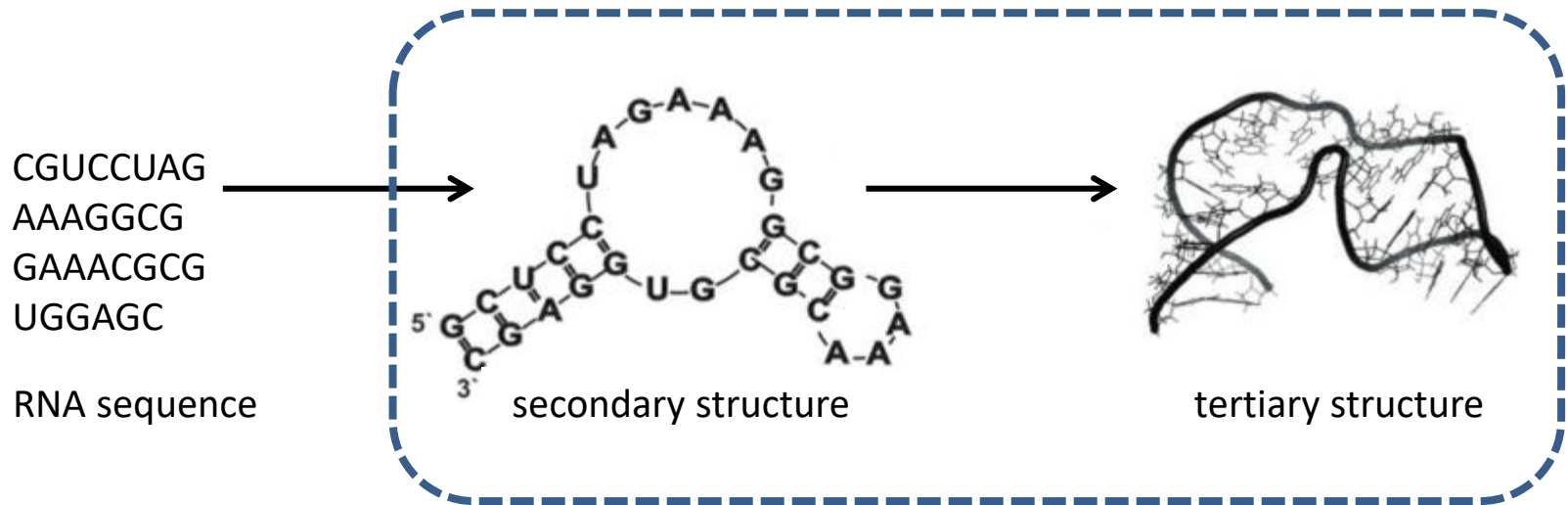
```
#tRNA(Phe), yeast (Saccharomyces Scerevisiae)
>strand1
gCGGAUUUAgCUCAGuuGGGAGAGCgCC
```

Popenda et al., *NAR*, 2008

Popenda et al., *BMC Bioinformatics*, 2010



# RNAComposer: 3D structure prediction



## Idea

Knowledge-based system deriving from comparative modeling but overcoming typical limitations of the other methods in the stream (no templates required from a user, no structural alignment).

## Result

Building atomic-resolution 3D-models of RNAs based on their secondary structures (and / or sequences) using the database of 3D RNA fragments (RNA FRABABE).

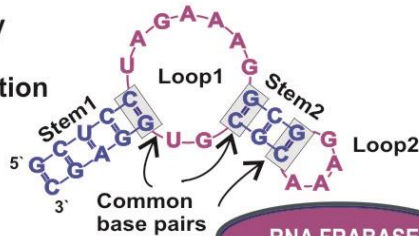
# RNAComposer method outline

## Input Data

GCUCCUAGAAAAGGCGGAAACGCGUGGAGC  
 ((((((.....(((.....))))..))))))

## RNA structure machine translation

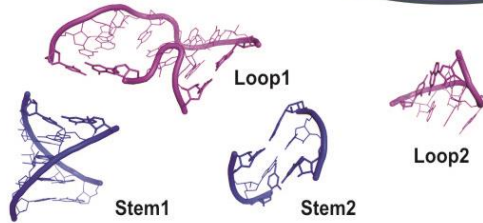
### Secondary structure fragmentation



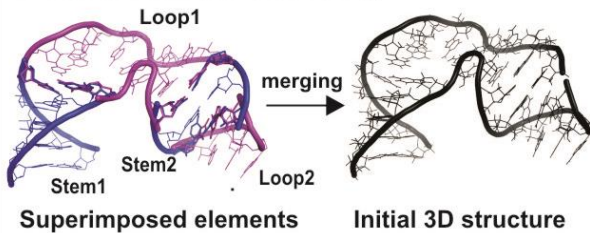
RNA FRABASE

structure elements dictionary

### 3D elements preparation



### Initial 3D structure building



### 3D structure refinement



1. *Optional secondary structure prediction* (*RNAstructure, RNAfold, CONTRAfold*)
2. **Validation** of the input data (provided / predicted secondary structure)
3. Secondary structure **fragmentation** (based on graph representation of RNA secondary structure)
4. **Searching** the RNA FRABASE database of known structures for matching 3D fragments
5. Fragment **modifications** (if necessary)
6. Fragment **assembly**
7. **Minimization** of the complete structure due to the energy and structural parameters (i.a. XPLOR, CYANA)



http://rnacomposer.cs.put.poznan.pl/

# RNACOMPOSER

Automated RNA Structure 3D Modeling Server

Home  
Tools  
Help  
About  
References  
Links  
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User ID:

Password:

[Forgot your password?](#)

[Create an account](#)

You are **49970**. visitor.

Visitors online: **4**

Supported by:



Department of Structural Chemistry and  
Biology of Nucleic Acids & Department  
of Bioinformatics, Institute of Bioorganic  
Chemistry, Polish Academy of Sciences



Institute of Computing Science, Poznan  
University of Technology

Welcome to RNAComposer, a fully automated RNA structure modeling server. (Mirror site: [rnacomposer.ibch.poznan.pl](http://rnacomposer.ibch.poznan.pl))

The RNAComposer system offers a new user-friendly approach to the fully automated prediction of large RNA 3D structures. The method is based on the machine translation principle and operates on the [RNA FRABASE](#) database acting as the dictionary relating RNA secondary structure and tertiary structure elements.

#### RNAComposer works in two modes:

- **interactive mode** - allows to work on one RNA molecule of interest at a time; its use is limited up to 500 nt residues and results in a single 3D-RNA structure model. Input your RNA sequence and secondary structure ([Example 1](#) and [Example 2](#)) or sequence only ([Example 3](#)). Example 3 is offered for introductory purposes.

- **batch mode** - is designed for large-scale automated modeling of RNA structures up to 500 nt residues, based on user-defined RNA secondary structures. As an input a set of up to 10 RNA sequences can be used. This mode is available only for registered users.

#### You are in interactive mode

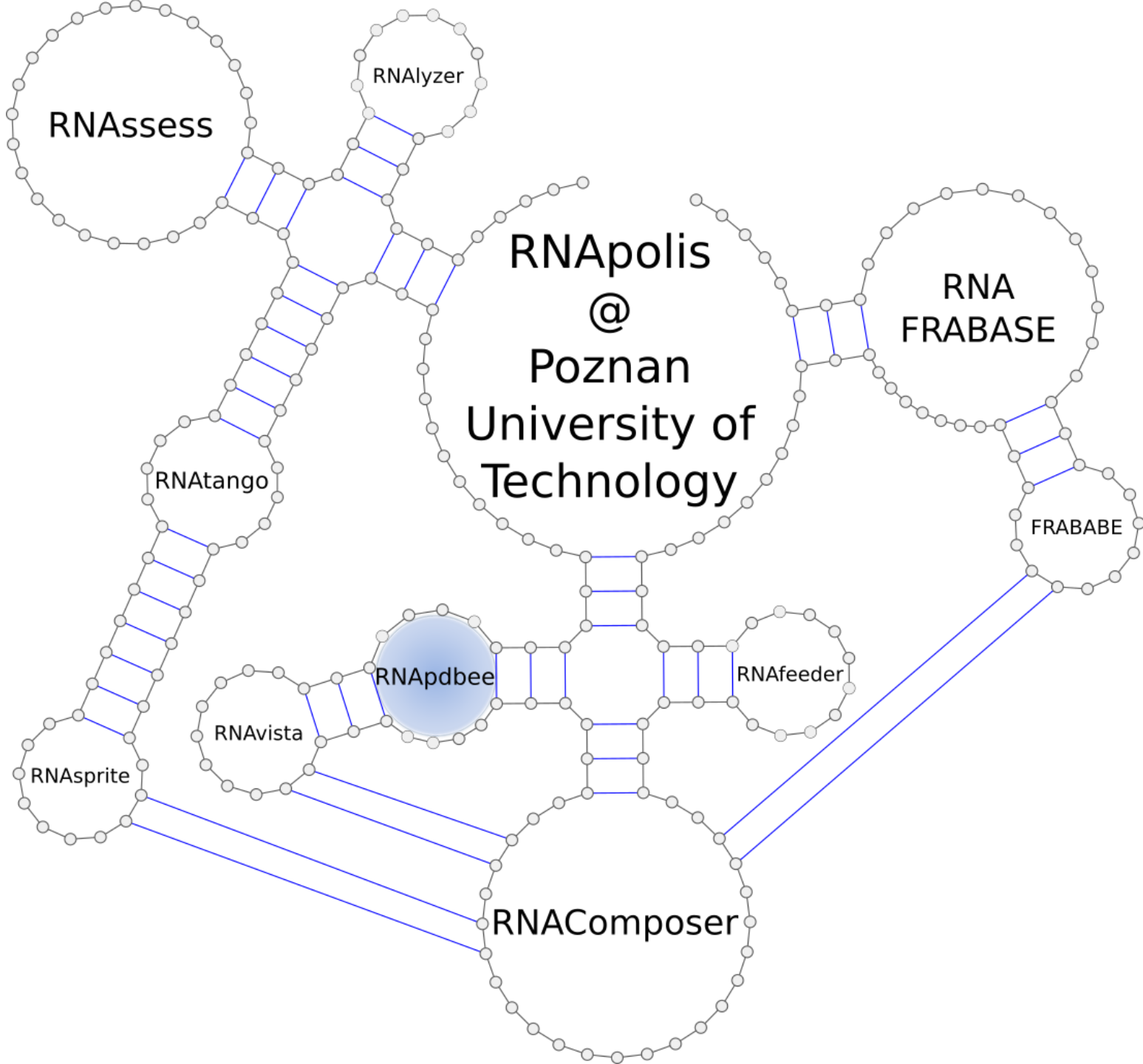
Enter RNA sequence and secondary structure in dot-bracket format ([Example 1](#) and [Example 2](#)) or sequence only ([Example 3](#)). A maximum sequence length is limited to 500 residues.

Load example: [1](#) [2](#) [3](#)

```
#HIV-2 DIS RNA hairpin  
>example1  
CCCCAAGCUAUGCAACCUUAUGGUCCUGUGGGAAGGGGA  
(((...((...))..((...)).(((...)))..)))..
```

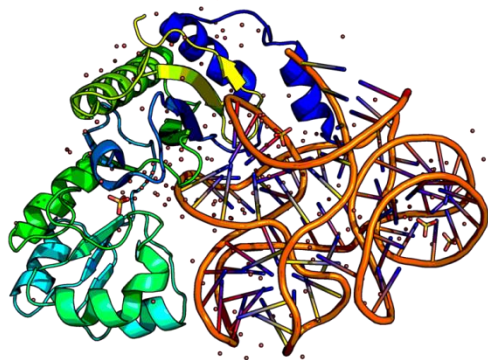
Email results to:

Popenda et al., *NAR*, 2012

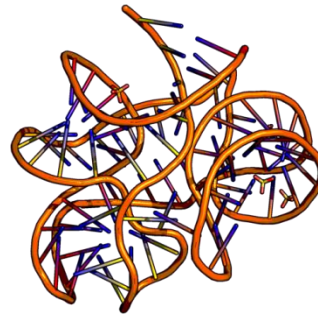


# RNApdbee: secondary structure from PDB files

Input (PDB id/ file)



➔  
Data  
filtering

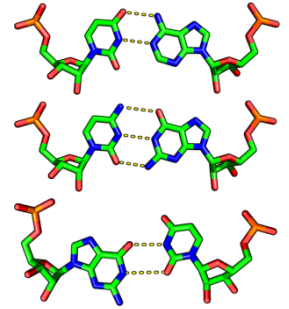


➔  
Base pair  
retrieval:  
RNAView,  
MC-Annotate,  
x3DNA/DSSR

```

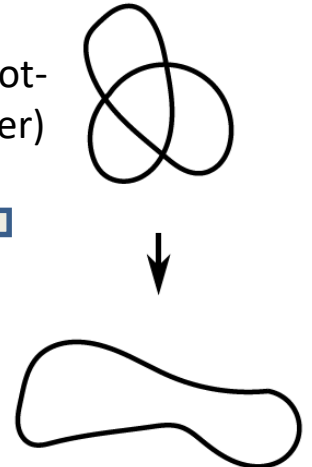
1 G 80
1 G 79
3 G 78
4 A 77
5 U 0
6 G 75
...

```



⬇️  
Temporary  
structure  
unknotting

Topology  
encoding (dot-  
bracket-letter)

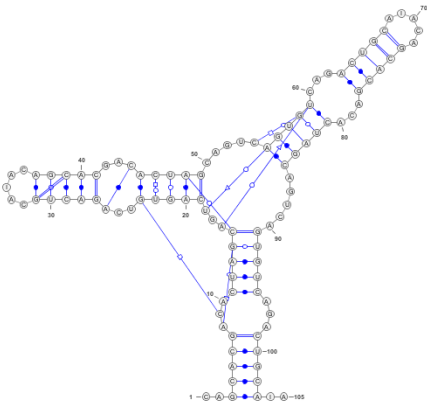


Structure  
visualization:  
Pseudoviewer,  
VARNA  
⬅️

```

GGGAUGCUGUAGGAUAGGUGG
GAGCCUGUGAACCCCGCCU
CCGGGUGGGGGGAGGCGCC
GGUGAAAUACCACCCUCCCC
((( (. . . . . [ . . ((( (
. . ((( . . . . . ((( ((( (
. . . . . ) . . . . . ) . . . . .
. . . . . ] . . . . . ) . . . . .

```



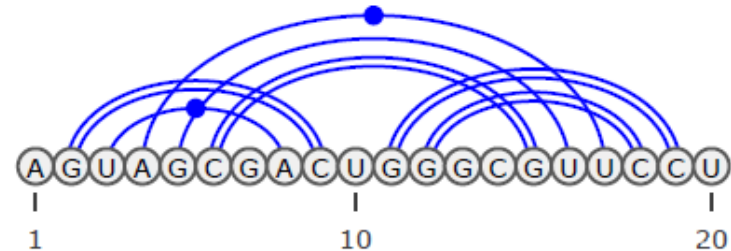
Output  
(textual & graphical)

# RNApdbee: pseudoknot order

**Pseudoknot order** - min number of base pair set decompositions that result in obtaining nested structure

## Pseudoknot order determination:

1. Unknot the structure iteratively (Elimination Gain heuristics)
2. Count the number of conflicts (=pseudoknot order) between paired regions

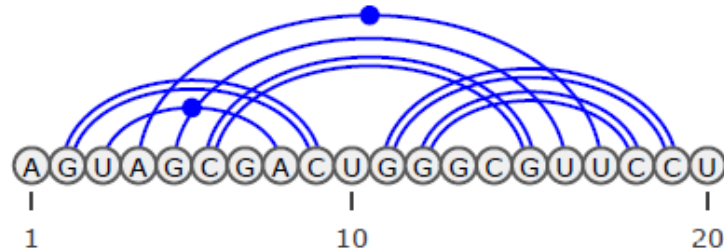


## Pseudoknot order encoding:

Pseudoknot order	1st	2nd	3rd	4th	5th	6th	7th	8th
Text annotation (brackets & letter)	[]	{}	<>	Aa	Bb	Cc	Dd	Ee
Graphical annotation (colours)	<span style="background-color: green; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: darkblue; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: darkred; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: purple; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: steelblue; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: olive; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: magenta; width: 20px; height: 15px; display: inline-block;"></span>	<span style="background-color: limegreen; width: 20px; height: 15px; display: inline-block;"></span>

# RNApdbee: where is pseudoknot?

Our assumption: minimize the number of pseudoknotted pairs

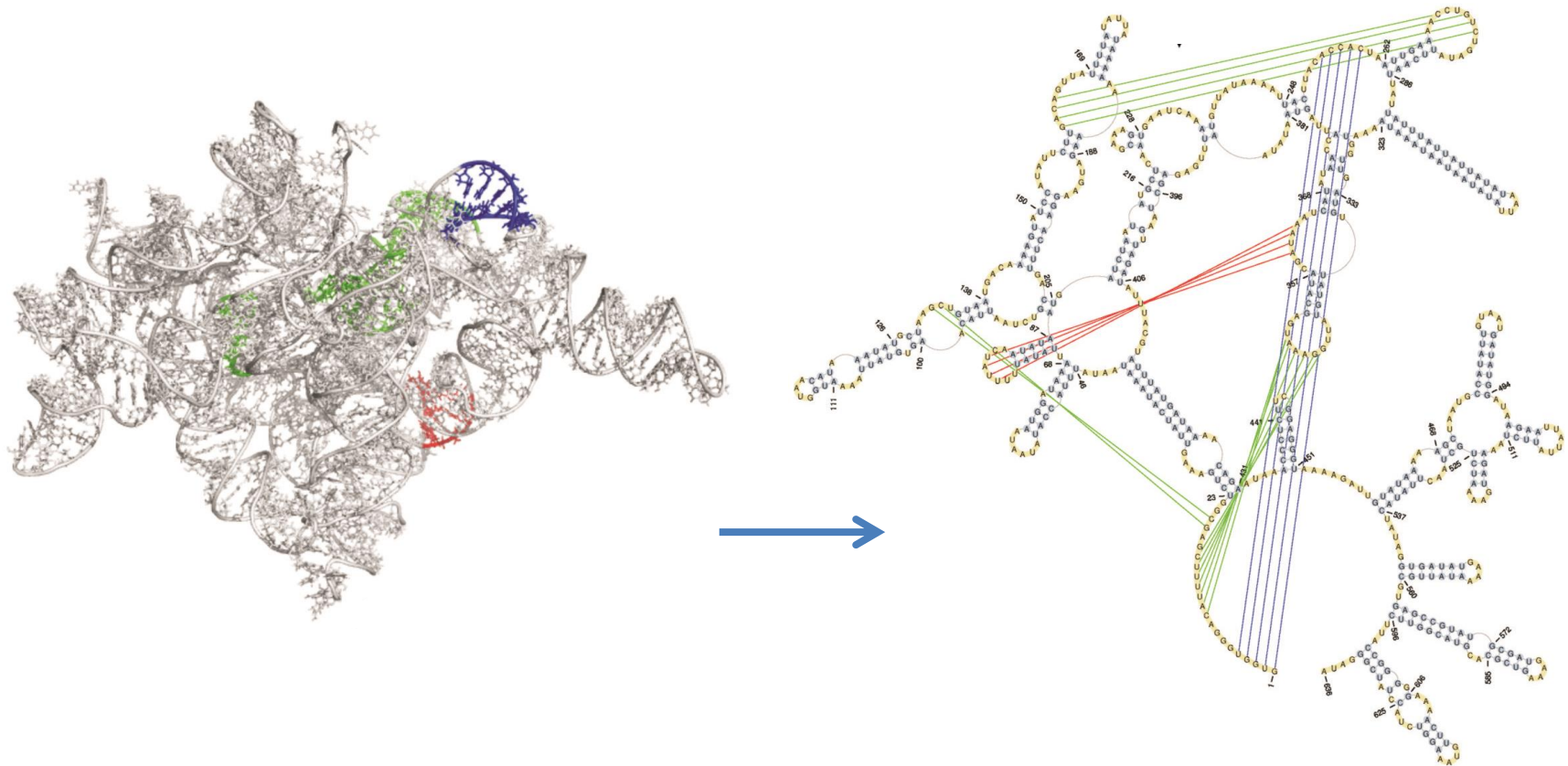


1	A	0	11	G	19
2	G	9	12	G	18
3	U	8	13	G	0
4	A	17	14	C	0
5	G	16	15	G	6
6	C	15	16	U	5
7	G	0	17	U	4
8	A	3	18	C	12
9	C	2	19	C	11
10	U	0	20	U	0

AGUAGCGACUGGGCGUUCCU  
 .((( [[[ [.)].((..]]] ))).

AGUAGCGACUGGGCGUUCCU  
 .[[((( (.]]].[[[.))]]].

# RNApdbee: example



# RNAppdbee

RNA secondary structure extraction from PDB files

- Home
- Help
- About
- Citations
- Links
- Contact Us

Welcome to RNAppdbee, a webserver to derive secondary structures from pdb files of knotted and unknotted RNAs.

RNAppdbee runs according to the following scenarios:

- in "3D → (...)" the secondary structure of RNA is derived from its tertiary structure provided in pdb file,
- in "2D → (...)" the secondary structure topology of RNA is derived from base-pair list provided in BPSEQ or CT.

In both scenarios, the resulting secondary structure encoded in dot-bracket, BPSEQ and CT is immediately released together with a graphical image (if checked).

3D → (...)

2D → (...)

## 1) Upload RNA pdb file:

- from PDB
- from local disk
- from example

Show file contents

Reset

PDB id

Get

Browse...

1 2 3 4

Data uploaded from: - (no file selected)

## 2) Identify base-pairs using:

and include non-canonical ones:

- RNAView
- MC-Annotate
- 3DNA/DSSR  Analyse helices
- in text and graphical representation
- in graphical representation only
- do not include

## 3) Generate graphical image using: (Note)

- Pseu
- VARN
- No in

4) Run

You are 3350 visitor  
Visitors online: 1

Supported by:

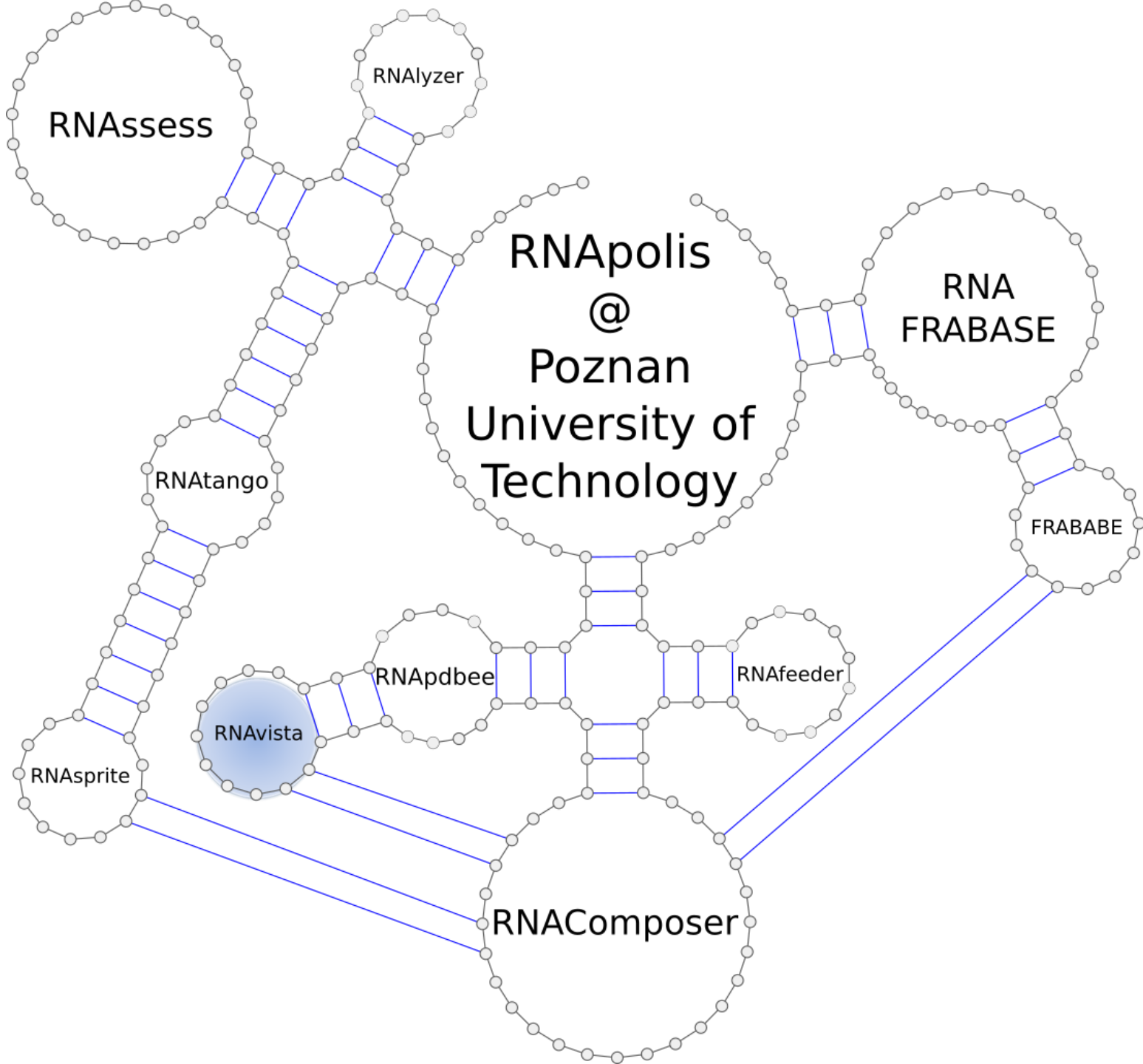


Institute of Computing Science, Poznan  
University of Technology



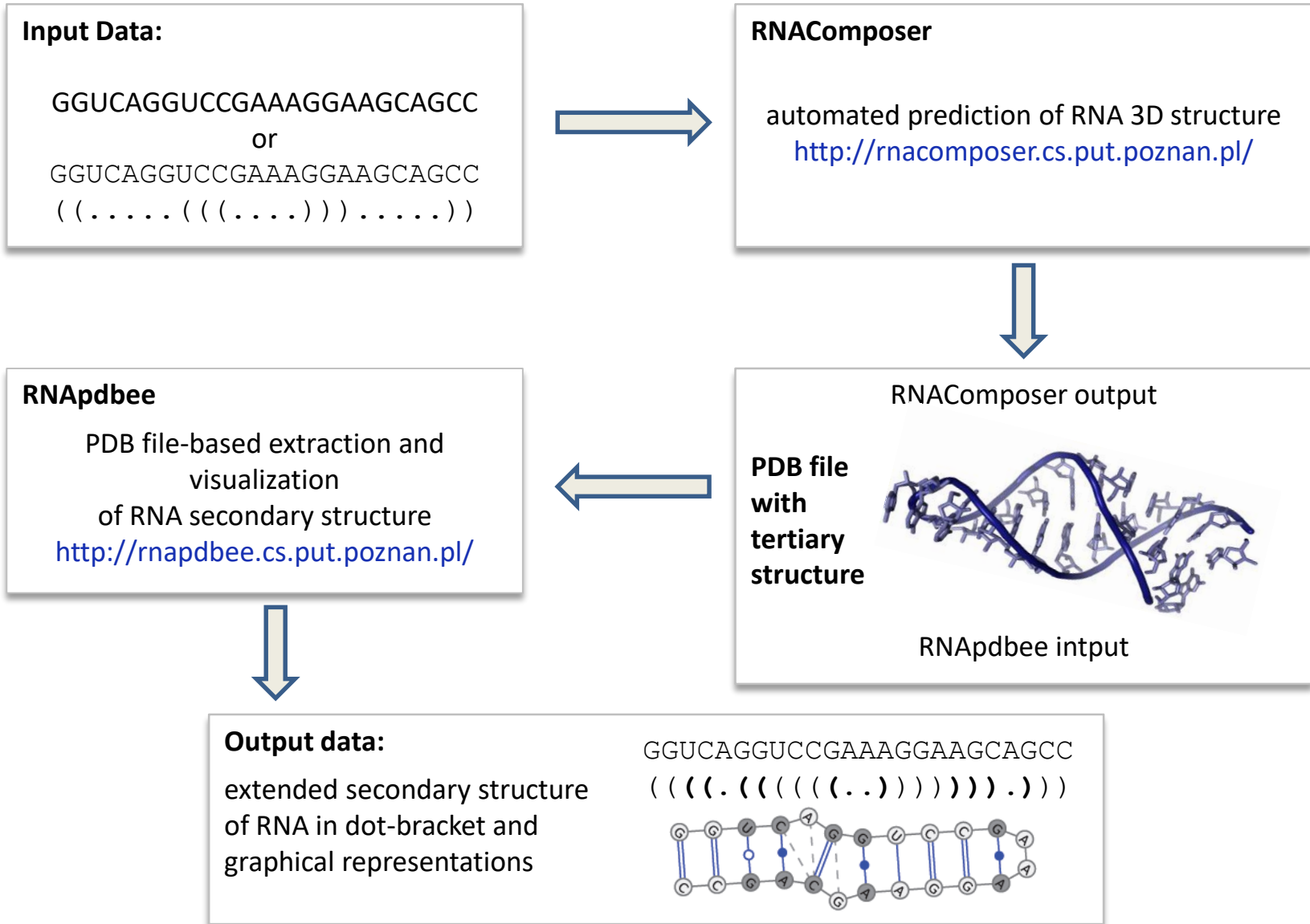
Department of Structural Chemistry and  
Biology of Nucleic Acids & Department of  
Bioinformatics, Institute of Bioorganic  
Chemistry, Polish Academy of Sciences

Antczak et al., *NAR*, 2014



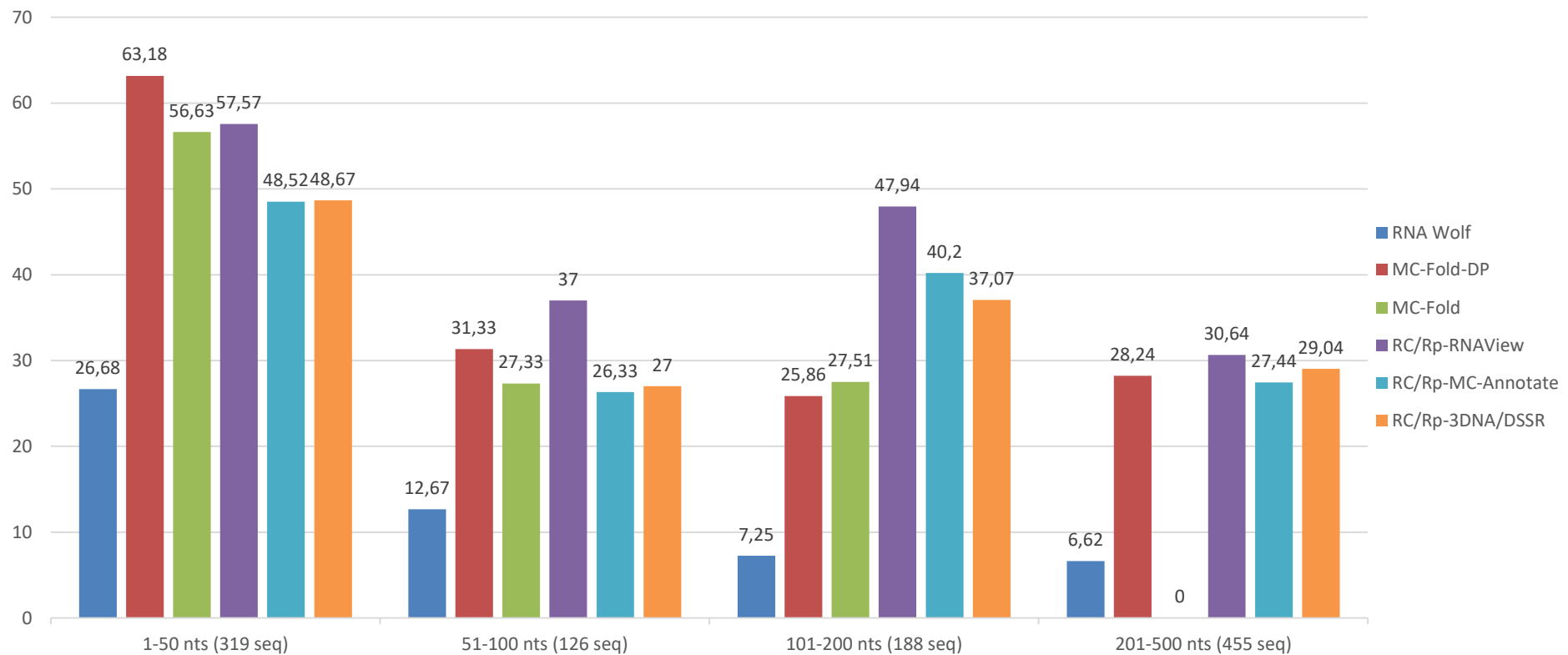


# RNAvista: extended secondary structure assessment



# RNAvista: preliminary tests

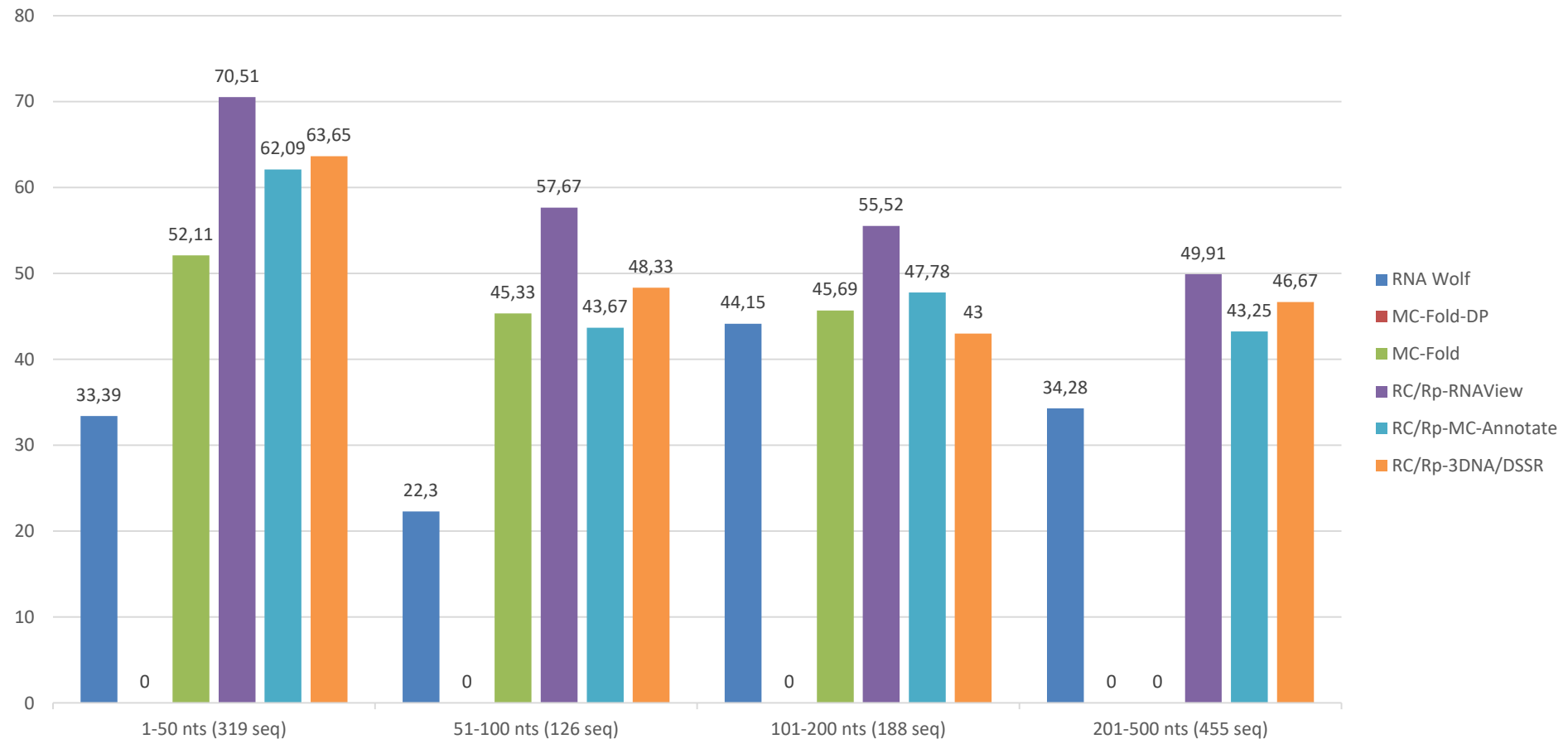
% of correctly predicted non-canonical base pairs present in the reference structures  
(non-canonical bps predicted from sequence)



Benchmark set: 1088 structures from RNA STRAND (with >2 non-canonical bps)

# RNAvista: preliminary tests

% of correctly predicted non-canonical base pairs presented in the reference structures  
(non-canonical bps predicted from canonical secondary structure)



Benchmark set: 1088 structures from RNA STRAND (with >2 non-canonical bps)

# People in RNAPolis

---



## COMPUTATIONAL...

Maciej Antczak

Jacek Blazewicz

Marek Blazewicz (left)

Piotr Lukasiak

Tomasz Ratajczak

Agnieszka Rybarczyk

Marta Szachniuk

Natalia Szostak

Tomasz Zok

## ...BIOLOGY

Ryszard W. Adamiak

Mariusz Popenda

Katarzyna J. Purzycka