

SUPPLEMENTARY MATERIAL

RNAPdbec 2.0: multifunctional tool for RNA structure annotation

Tomasz Zok^{1,2}, Maciej Antczak¹, Michal Zurkowski¹, Mariusz Popena³, Jacek Blazewicz^{1,3},
Ryszard W. Adamiak^{1,3} and Marta Szachniuk^{1,3*}

¹Institute of Computing Science & European Centre for Bioinformatics and Genomics, Poznan University of Technology,
Piotrowo 2, 60-965 Poznan, Poland

²Poznan Supercomputing and Networking Center, Jana Pawla II 10, 61-139 Poznan, Poland

³Institute of Bioorganic Chemistry, Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznan, Poland

*corresponding author: marta.szachniuk@cs.put.poznan.pl

WEB SITE: <http://rnapdbec.cs.put.poznan.pl/>

TABLE OF CONTENTS

Figure S1. Diagrams of the 3D structure-derived secondary structure of RNA aptamer (PDB id: 4Q9Q) generated by (a) RNApdbee 1.0 and (b) RNApdbee 2.0 that applies a new function which skips isolated base-pair impact while drawing structure topology.	3
Figure S2. Secondary structure of vitamin B12 RNA aptamer (PDB id: 1DDY) strands drawn by VARNA-based procedure of RNApdbee 2.0.	4
Figure S3. Results of RNApdbee 2.0 function <i>Identify structural elements</i> with pseudoknots treated as unpaired residues applied to one strand of vitamin B12 RNA aptamer (PDB id: 1DDY, chain A), and their PyMOL visualization.	5
Figure S4. Results of RNApdbee 2.0 function <i>Identify structural elements</i> with pseudoknots treated as paired residues applied to one strand of vitamin B12 RNA aptamer (PDB id: 1DDY, chain A), and their PyMOL visualization.	6
Figure S5. Quadruplex 3D structure of oxytricha telomeric DNA (PDB id: 1JPQ) and its secondary structure diagram given by RNApdbee 2.0.....	7

Figure S1. Diagrams of the 3D structure-derived secondary structure of RNA aptamer (PDB id: 4Q9Q) generated by (a) RNApdbee 1.0 and (b) RNApdbee 2.0 that applies a new function which skips isolated base-pair impact while drawing structure topology.

gGACGCGACCGAAAUGGUGAAGGACGGGUCCAGUGCGAAACACGCACUGUUGAGUAGAGUGUGAGCUCGUAACUGGUCGCGUC
. (((((((((... (((

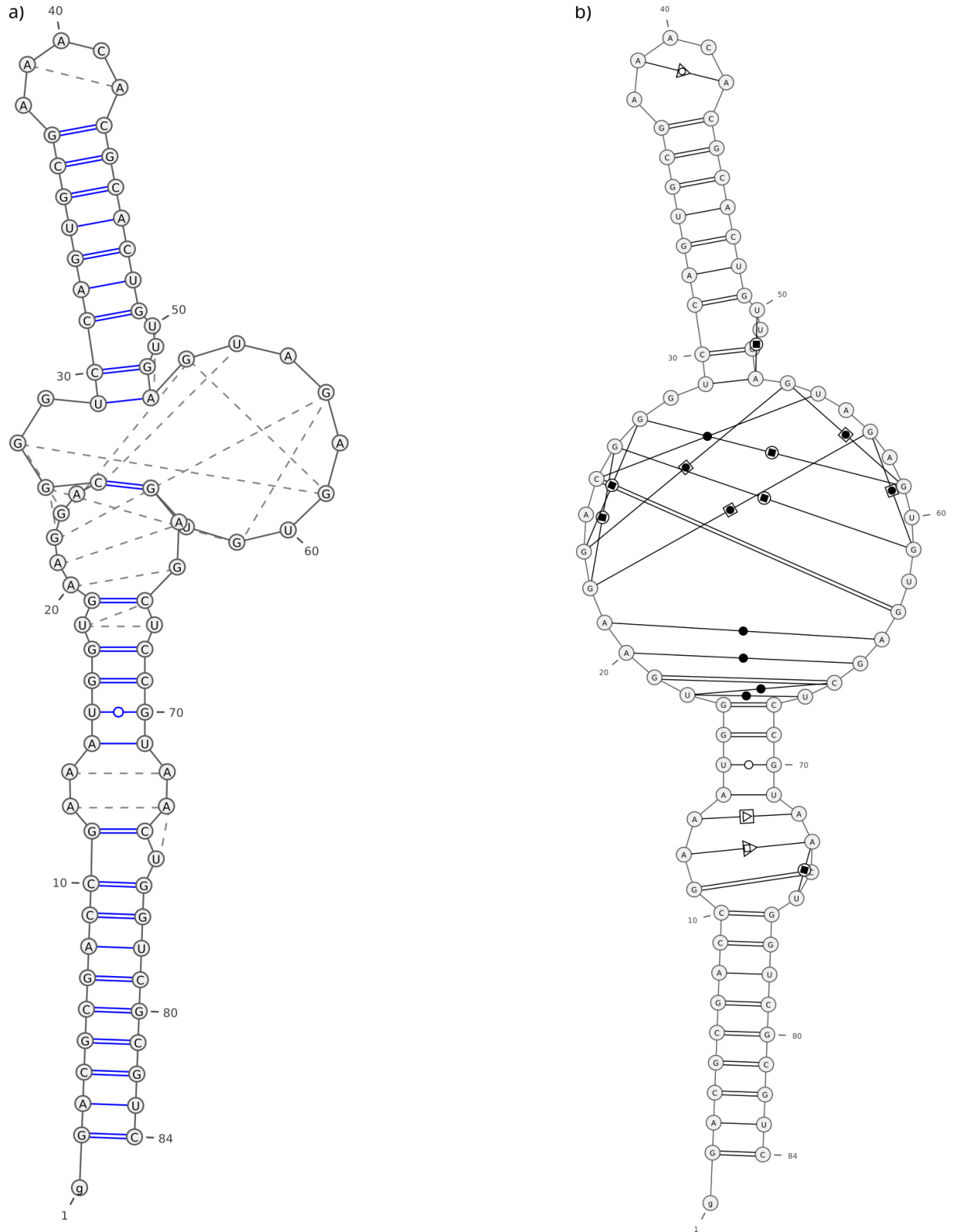


Figure S2. Secondary structure of vitamin B12 RNA aptamer (PDB id: 1DDY) strands drawn by VARNA-based procedure of RNAppdbec 2.0.

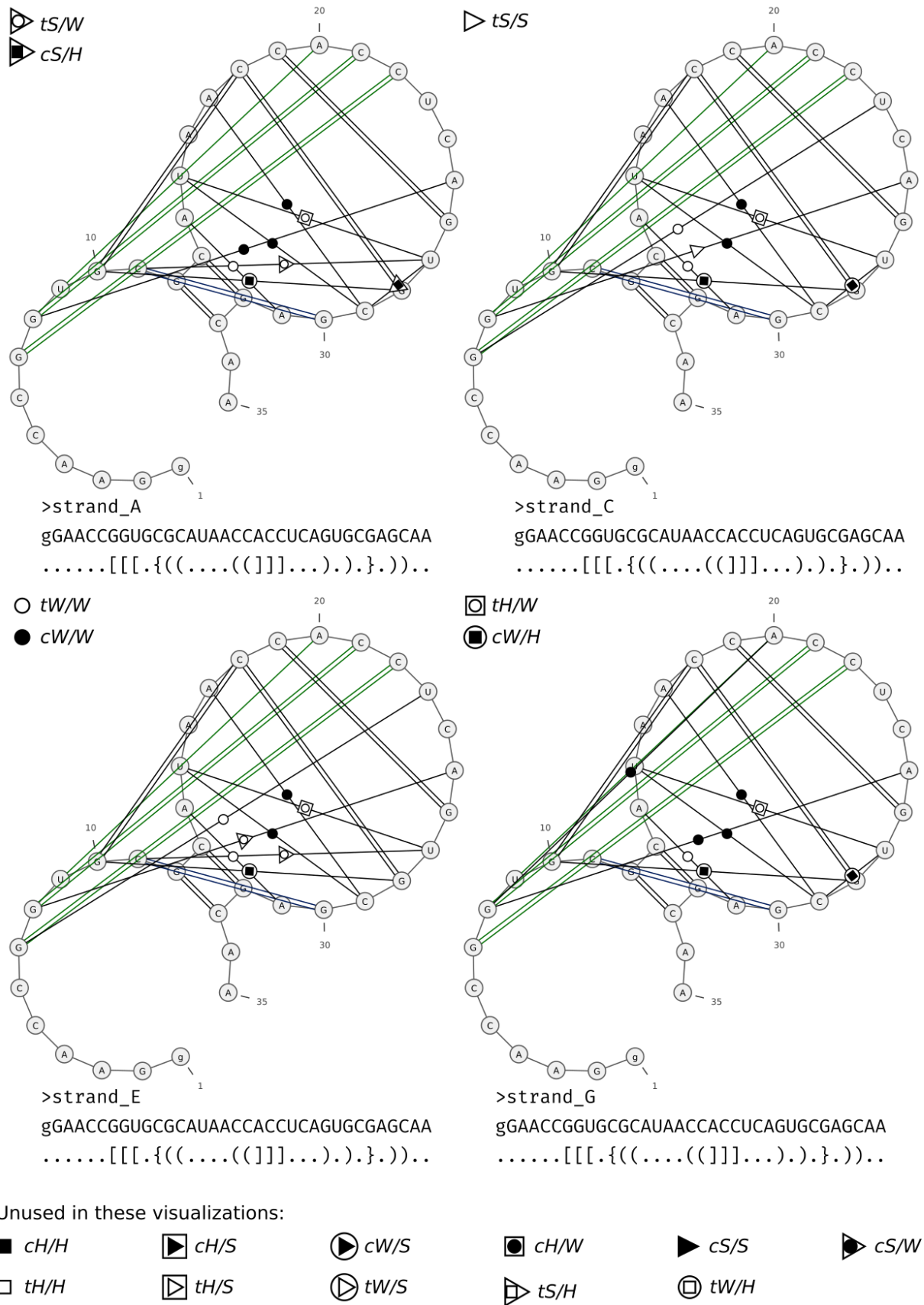


Figure S3. Results of RNApdbee 2.0 function *Identify structural elements* with pseudoknots treated as unpaired residues applied to one strand of vitamin B12 RNA aptamer (PDB id: 1DDY, chain A), and their PyMOL visualization.

```

Stem D1 A.12 A.13 GC (( RY A.32 A.33 GC )) RY

Loop L1 A.13 A.18 CAUAAC (... ( YRYRRY A.28 A.32 GCGAG ).).) RYRRR
Loop L2 A.18 A.19 CC (( YY A.26 A.28 GUG ).) RYR
Loop L3 A.19 A.26 CACCUCAG (]]]...) YRYYYRR

Single strand 5' SS5p A.1 A.12 gGAACCGGUGCG .....[[[.({ YRRRYRRYR
Single strand 3' SS3p A.33 A.35 CAA ).. YRR

```

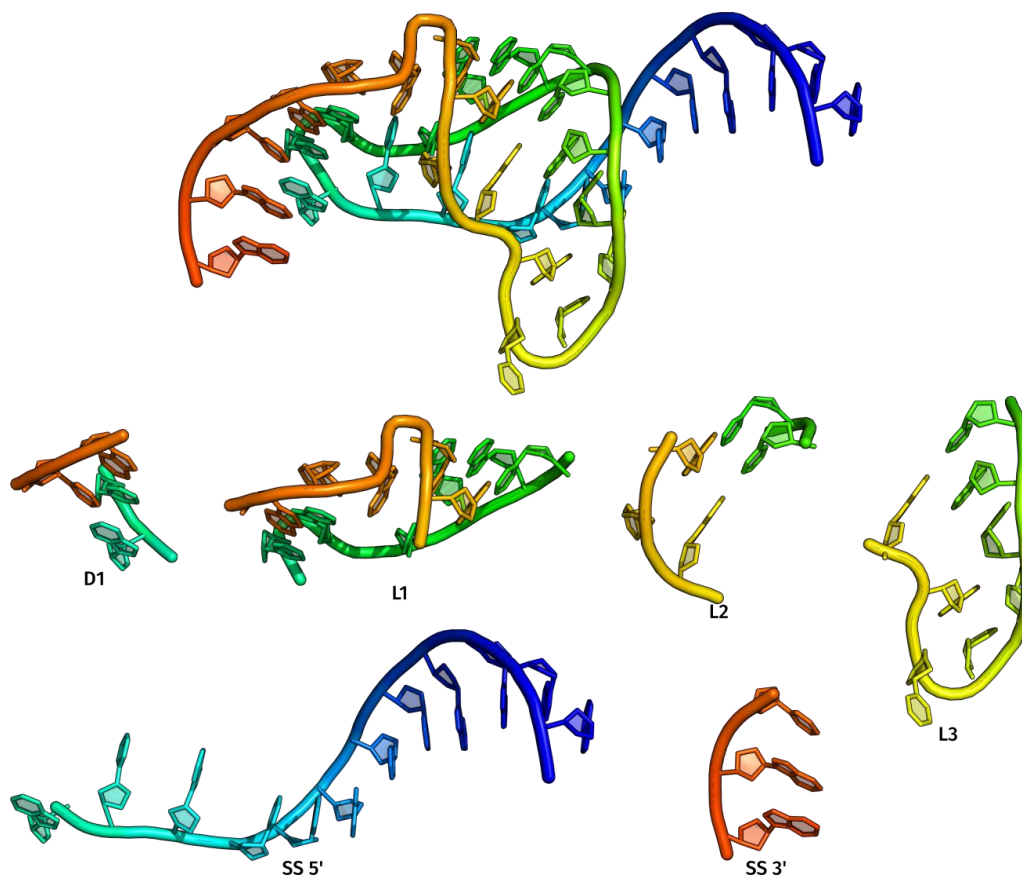


Figure S4. Results of RNAPdbec 2.0 function *Identify structural elements* with pseudoknots treated as paired residues applied to one strand of vitamin B12 RNA aptamer (PDB id: 1DDY, chain A), and their PyMOL visualization.

```

Stem D1 A.7 A.9 GGU [[[ RRY A.20 A.22 ACC ]]] RYY
Stem D2 A.12 A.13 GC (( RY A.32 A.33 GC )) RY

Loop L1 A.13 A.18 CAUAAC (... ( YRYRRY A.28 A.32 GCGAG ).).) RYRRR
Loop L2 A.18 A.19 CC (( YY A.26 A.28 GUG ).) RYR
Loop L3 A.19 A.26 CACCUCAG (]]]...) YRYYYRR

Single strand SS1 A.9 A.11 UGC [.{ YRY
Single strand SS2 A.13 A.18 CAUAAC (... ( YRYRRY
Single strand SS3 A.22 A.26 CUCAG ]...) YYRR
Single strand SS4 A.26 A.28 GUG ).) RYR
Single strand SS5 A.28 A.30 GCG ).) RYR
Single strand SS6 A.28 A.32 GCGAG ).).) RYRRR
Single strand SS7 A.30 A.32 GAG }.) RRR

Single strand 5' SS5p A.1 A.7 gGAACCG .....[ YRRRYR
Single strand 5' SS5p A.1 A.12 gGAACCGUGCG .....[[[.{( YRRRYRRYR

Single strand 3' SS3p A.33 A.35 CAA ).. YRR

```

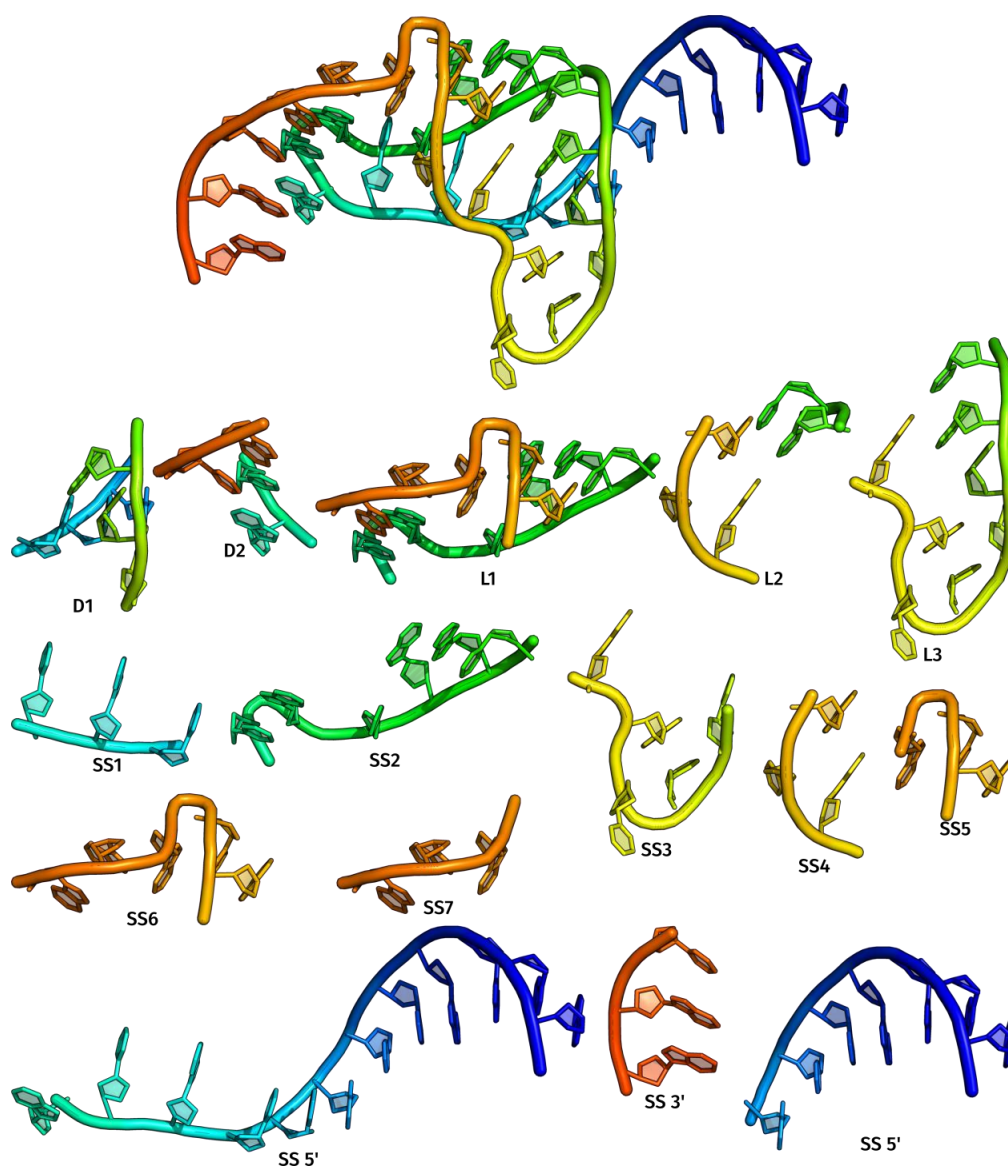


Figure S5. Quadruplex 3D structure of oxytricha telomeric DNA (PDB id: 1JPQ) and its secondary structure diagram given by RNApdbee 2.0.

