- 1. W narzędziu XRNA porównujemy struktury używając 4 konfiguracji wprowadzoych danych: run with ETRNA pdb, run with ETRNA pdb and all basepairs, run with W. Scott Hammerhead Ribozyme oraz normal run.
- 2. Porównywanane struktury wyrzucają identyczne dane przykład z symulacji dla 2nbx:
- a) run with ETRNA pdb 1 chains, 22 bondpairs, (5 = helices*2):

- label	file:
AETN	1
A ETNI	2

C G AETN 2

AETN 3 С

AETN 4 G

G AETN 5

AETN 6 G

AETN 7 G

AETN 8 U

G AETN 9

AETN 10 G

AETN 11 Α

AETN 12 G

AETN 13 C

Α AETN 14

AETN 15 G

AETN 16 C

C AETN 17

AETN 17A U

AETN 18 G

AETN 19 G

AETN 20 U

AETN 21 Α

AETN 22 G

AETN 23 C

AETN 24 U

C AETN 25

G AETN 26

AETN 27 U

C AETN 28

G AETN 29 AETN 30 G

G AETN 31

AETN 32 C

AETN 33 U

С AETN 34

AETN 35 Α

AETN 36 U AETN 37 Α

AETN	38	Α
AETN	39	С
AETN	40	С
AETN	41	С
AETN	42	G
AETN	43	Α
AETN	44	Α
AETN	45	G
AETN	46	G
AETN	47	U
AETN	48	C
AETN	49	G
AETN	50	U
AETN	51	C
AETN	52	G
AETN	53	G
AETN	54	U
AETN	55	U
AETN	56	C
AETN		Α
AETN	58	Α
AETN	59	Α
AETN	60	U
AETN	61	C
AETN	62	C
AETN	63	G
AETN	64	G
AETN	65	C
AETN	66	C
AETN	67	C
AETN	68	C
AETN	69	C
AETN	70	G
AETN	71	C
AETN	72	Α
AETN	73	Α
AETN	74	C
AETN	75	C

- base pair file:

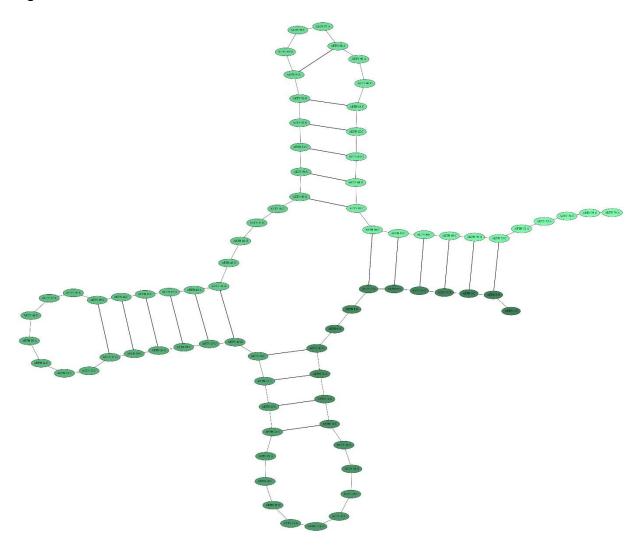
Α

AETN 76

1	AETN	2	GUA	AETN	71	CYT	XIX
2	AETN	3	CYT	AETN	70	GUA	XIX
3	AETN	4	GUA	AETN	69	CYT	XIX
4	AETN	5	GUA	AETN	68	CYT	XIX
5	AETN	6	GUA	AETN	67	CYT	XIX
6	ΔFTN	7	GHA	ΔFTN	66	CYT	XIX

8	AETN	10	GUA	AETN	25	CYT	XIX
9	AETN	11	ADE	AETN	24	URI	XX
10	AETN	12	GUA	AETN	23	CYT	XIX
11	AETN	13	CYT	AETN	22	GUA	XIX
14	AETN	26	GUA	AETN	44	ADE	VIII
15	AETN	27	URI	AETN	43	ADE	XX
16	AETN	28	CYT	AETN	42	GUA	XIX
17	AETN	29	GUA	AETN	41	CYT	XIX
18	AETN	30	GUA	AETN	40	CYT	XIX
19	AETN	31	GUA	AETN	39	CYT	XIX
21	AETN	49	GUA	AETN	65	CYT	XIX
22	AETN	50	URI	AETN	64	GUA	XXVIII
23	AETN	51	CYT	AETN	63	GUA	XIX
24	AETN	52	GUA	AETN	62	CYT	XIX
25	AETN	53	GUA	AETN	61	CYT	XIX
26	AETN	54	URI	AETN	58	ADE	XXIV

- grafika:



b) run with ETRNA pdb and all basepairs - 1 chains , 26 bondpairs , (9 = helices*2):

.,		
-label	file:	
AETN	1	С
AETN	2	G
AETN	3	С
AETN	4	G
AETN	5	G
AETN	6	G
AETN	7	G
AETN	8	U
AETN	9	G

AETN 10 G AETN 11 A

AETN 12 G AETN 13 C

AETN 14 A AETN 15 G

AETN 16 C AETN 17 C AETN 17A U

AETN 18 G AETN 19 G

AETN 20 U AETN 21 A

AETN 22 G AETN 23 C

AETN 24 U AETN 25 C

AETN 26 G AETN 27 U

AETN 28 C AETN 29 G AETN 30 G

AETN 30 G

AETN 32 C AETN 33 U

AETN 34 C

AETN 35 A AETN 36 U

AETN 37 A

AETN 38 A

AETN 39 C AETN 40 C

AETN 40 C AETN 41 C

AETN 41 C

AETN 43 A

```
AETN 44
            Α
AETN 45
            G
AETN 46
            G
AETN 47
            U
            C
AETN 48
AETN 49
            G
AETN 50
            U
AETN 51
            C
AETN 52
            G
AETN 53
            G
AETN 54
            U
AETN 55
            U
AETN 56
            C
AETN 57
            Α
AETN 58
            Α
AETN 59
            Α
AETN 60
            U
            C
AETN 61
            C
AETN 62
AETN 63
            G
AETN 64
            G
AETN 65
            C
            C
AETN 66
            C
AETN 67
            C
AETN 68
AETN 69
            C
AETN 70
            G
AETN 71
            C
AETN 72
            Α
AETN 73
            Α
AETN 74
            C
            C
AETN 75
AETN 76
            Α
- base pair file:
             2
                  GUA
                        AETN
1
      AETN
                               71
2
      AETN
             3
                  CYT
                        AETN
                               70
```

3

4

5

6

7

8

9

10

11

12

AETN

4

5

6

7

8

10

11

12

13

15

GUA

GUA

GUA

GUA

URI

GUA

ADE

GUA

CYT

GUA

AETN

69

68

67

66

14

25

24

23

22

48

CYT

GUA

CYT

CYT

CYT

CYT

ADE

CYT

URI

CYT

GUA

CYT

XIX

XIX

XIX

XIX

XIX

XIX

XXIV

XIX

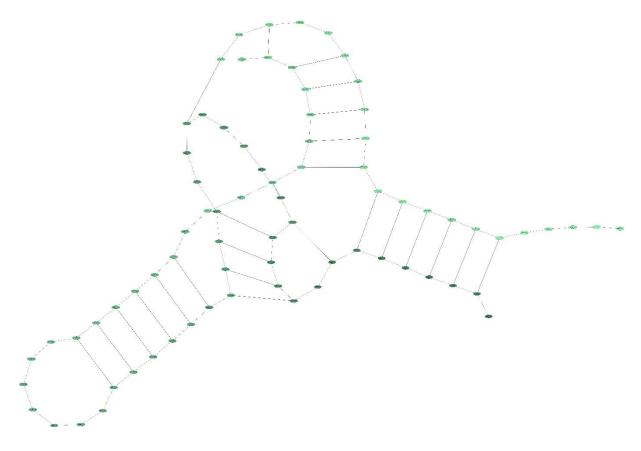
XX

XIX

XIX XXII

```
AETN
13
      AETN
                  GUA
                                    CYT
                                          XIX
             19
                               56
14
      AETN
             22
                  GUA
                        AETN
                               46
                                    GUA
                                          VII_HW
15
      AETN
                  GUA
                        AETN
                               44
                                    ADE
                                          VIII
             26
16
      AETN
             27
                  URI
                        AETN
                               43
                                    ADE
                                          XX
      AETN
             28
                  CYT
                        AETN
                                    GUA
                                          XIX
17
                               42
                  GUA
                        AETN
18
      AETN
             29
                               41
                                    CYT
                                          XIX
19
      AETN
             30
                  GUA
                        AETN
                               40
                                    CYT
                                          XIX
20
      AETN
             31
                  GUA
                        AETN
                               39
                                    CYT
                                          XIX
21
      AETN
             49
                  GUA
                        AETN
                               65
                                    CYT
                                          XIX
                                          XXVIII
22
      AETN
             50
                  URI
                        AETN
                               64
                                    GUA
23
      AETN
                  CYT
                        AETN
                                    GUA
                                          XIX
             51
                               63
24
      AETN
             52
                  GUA
                        AETN
                               62
                                    CYT
                                          XIX
25
                                    CYT
                                          XIX
      AETN
             53
                  GUA
                        AETN
                               61
26
      AETN
                  URI
                               58
                                    ADE
                                          XXIV
             54
                        AETN
```

- grafika:



c) run with W. Scott Hammerhead Ribozyme - 2 chains, 23 bondpairs, (11 = helices*2):

- label file:

Α	2	G
Α	3	Α
Α	4	U
Α	5	G

A 6 U A 7 A 8 C U A 7 A 8 A 9 U A 10 A 11 C C A 13 A 14 G C U G A 15 A 16 A 17 A 18 A 19 G A 21 A 22 A 23 A 24 A 25 A 26 A 27 A 28 A 29 A A 30 A 31 A 32 G A 33 G A 34 A 35 G A 37 A 38 A A 39 A A 40 A 31 A 32 G A 33 G A 34 A 35 G A 37 A 38 A A 39 A A 40 A 41 G A 42 C A 41 G A 42 C A 43 B 1 G G B 8 B 10 G G G G G G G G G G G G G G G G G G	_	_	
A 8 C U A 9 U A 10 A 11 C C A 11 A 12 C A 13 A A 14 G A 15 C U A 16 A 17 A 18 A 19 U A 20 G A 21 A 22 G A 23 C C A 26 A 27 A 28 A 29 A 30 U A 21 A 22 G A 27 A 28 A 31 A 32 G A 31 A 32 G A 31 A 32 G A 33 G A 34 A 35 G A 37 A 38 A A 39 A A 30 C C A 37 A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C G B 1 G G B 1 G G G G G G G G G G G G G		6	U
A 8 C U A 9 U A 10 A 11 C C A 11 A 12 C A 13 A A 14 G A 15 C U A 16 A 17 A 18 A 19 U A 20 G A 21 A 22 G A 23 C C A 26 A 27 A 28 A 29 A 30 U A 21 A 22 G A 27 A 28 A 31 A 32 G A 31 A 32 G A 31 A 32 G A 33 G A 34 A 35 G A 37 A 38 A A 39 A A 30 C C A 37 A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C G B 1 G G B 1 G G G G G G G G G G G G G	Α	7	Α
A 9 U A 10 A 11 C A 11 C A 12 C A 13 A 14 G A 15 C A 16 A 17 A 18 A 19 U A 20 G A 21 A 22 G A 23 U A 24 C A 25 A 26 A 27 A 28 A 29 A 30 U A 31 A 32 G A 33 G A 34 A 35 G A 37 A A 38 A A 39 A A 30 C A 31 A 32 G A 31 A A 32 A A A 3	Α	8	С
A 10 A 11 C A 12 C A 13 A A 14 G A 15 C A 16 U A 17 G A 18 A A 19 U A 20 G A 21 A 22 G A 23 U A 24 C A 25 C A A 26 A 27 A A 28 A A 29 A A 30 U A 31 A A 32 G A 33 G A 34 A A 35 C A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B B 1 G B 2 G B B 3 G G B 5 C B B 5 C B B 7 C B B 9 G	Α	9	U
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		Α
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	11	С
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		С
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		Α
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Δ		G
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Δ	15	C
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	^		11
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	^	10	0
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	A		G
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	A		Α
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	А		U
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		G
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	21	Α
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	22	G
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	23	U
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	24	С
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		С
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	26	С
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		Α
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	28	Α
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Δ		Δ
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	٨		11
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	^	21	٨
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	^	21	A
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	A	32	G
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	A	33	G
A 36 G A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	34	Α
A 37 A A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		C
A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G			
A 38 A A 39 A A 40 C A 41 G A 42 C A 43 C B 1 G B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	37	Α
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	38	Α
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	39	Α
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		С
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α	41	G
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Α		C
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	Δ		C
B 2 G B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	R		G
B 3 C B 4 G B 5 U B 7 C B 8 U B 9 G	D D	2	6
B 8 U B 9 G		2	0
B 8 U B 9 G	D D	⊃	<u></u>
B 8 U B 9 G		4	
B 8 U B 9 G		5	Ū
B 9 G		7	
		8	
B 10 G			
	В	10	G

В	12	Α
В	13	U
В	14	С
В	15	С
В	16	Α
В	17	Α
В	18	U
В	19	С
В	20	D(

- base pair file:

- pa						
Α	2	G	В	19	С	XIX
Α	3	Α	В	18	U	XX
Α	5	G	В	14	С	XIX
Α	6	U	Α	28	Α	XXIV
Α	8	С	Α	26	С	XV
Α	9	U	В	12	Α	XX
Α	11	С	В	10	G	XIX
Α	12	С	В	9	G	XIX
Α	13	Α	В	8	U	XX
Α	14	G	В	7	С	XIX
Α	15	С	Α	20	G	XIX
Α	21	Α	Α	36	G	ΧI
Α	22	G	Α	35	С	XIX
Α	23	U	Α	34	Α	XX
Α	24	С	Α	33	G	XIX
Α	25	С	Α	32	G	XIX
Α	31	Α	В	13	U	XXIV
Α	39	Α	В	5	U	XX
Α	40	С	В	4	G	XIX
Α	41	G	В	3	С	XIX
Α	42	С	В	2	G	XIX
Α	43	С	В	1	G	XIX
В	15	С	Α	4	U	XVIII
	A A A A A A A A A A A A A A A A A A A	A 3 A 5 A 6 A 8 A 9 A 11 A 12 A 13 A 14 A 15 A 21 A 22 A 23 A 24 A 25 A 31 A 39 A 40 A 41 A 42 A 43	A 3 A A 5 G A 6 U A 8 C A 9 U A 11 C A 12 C A 13 A A 14 G A 15 C A 21 A A 22 G A 23 U A 24 C A 25 C A 31 A A 39 A A 40 C A 41 G A 42 C A 43 C	A 3 A B A 5 G B A 6 U A A 8 C A A 9 U B A 11 C B A 12 C B A 13 A B A 14 G B A 15 C A A 21 A A A 22 G A A 23 U A A 24 C A A 25 C A A 31 A B A 39 A B A 40 C B A 41 G B A 42 C B A 43 C B	A 3 A B 18 A 5 G B 14 A 6 U A 28 A 8 C A 26 A 9 U B 12 A 11 C B 10 A 12 C B 9 A 13 A B 8 A 14 G B 7 A 15 C A 20 A 21 A A 36 A 22 G A 35 A 23 U A 34 A 24 C A 33 A 25 C A 32 A 31 A B 13 A 39 A B 5 A 40 C B 4 A 41 G B 3 A 42 C B 2 A 43 C B 1	A 3 A B 18 U A 5 G B 14 C A 6 U A 28 A A 8 C A 26 C A 9 U B 12 A A 11 C B 10 G A 12 C B 9 G A 13 A B 8 U A 14 G B 7 C A 15 C A 20 G A 21 A A 36 G A 22 G A 35 C A 23 U A 34 A A 24 C A 33 G A 25 C A 32 G A 31 A B 13 U A 39 A B 5 U A 40 C B 4 G A 41 G B 3 C A 42 C B 2 G A 43 C B 1 G

- grafika:

Grafika się nie załadowała przy wielokrotnych próbach.

d) normal run:

Występuje błąd przy wielokrotnych próbach oraz różnorodnych plikach wejściowych – "problem with bp file, errcode23".

3. Narzędzie uznajemy więc za niepoprawnie działające dla próbowanych struktur drugorzędowych, co skutkuje również brakiem funkcjonalności. Dodatkową wadą jest fakt, że bardzo często się zawiesza, co prowadzi do uporczywego uzyskiwania danych.