

Electronic Supplementary Information for Prediction of DNA and RNA Structure with the NARES-2P Force Field and Conformational Space Annealing

Adam K. Sieradzan,^{*a,b} Łukasz Golon,^a and Adam Liwo^{a,b}

^a *Faculty of Chemistry, University of Gdańsk, 80-308 Gdańsk, Poland. Fax: +48 48 523-5012; Tel: +48 58 523 5142; E-mail: adams86@wp.pl*

^b *School of Computational Sciences, Korea Institute for Advanced Study, 85 Hoegiro, Dongdaemun-gu, Seoul 130-722, Republic of Korea.*

Constraints derived from the CyloFold server

In one of the simulations of PreQ1 Class II riboswitch from *Streptococcus pneumoniae* we used constraints based on the results of CyloFold server contact prediction. We used the CyloFold output directly with no further processing, thus if a particular contact was listed twice (e.g., 2 28 and 28 2), the constraint was twice as strong. The following pairs of nucleobases were subject to constraints:

2 28
3 27
4 26
5 25
6 24
7 23
8 22
9 21
15 57
16 56
17 55
18 54
19 53
20 52
22 8
23 7
24 6
25 5
26 4
27 3
28 2
29 1
39 49
40 48
41 47
42 46
47 41
48 40
49 39
50 38
53 19
54 18
55 17
56 16
57 15
58 14