**Supplementary Materials**

**Exploring dynamics of RNA molecules with multiscale Gaussian network model**

Shihao Wang, Weikang Gong, Xueqing Deng, Yang Liu, Chunhua Li\*

College of Life Science and Bioengineering, Beijing University of Technology, Beijing 100124, China

\*All correspondence should be addressed to Chunhua Li (E-mail: chunhuali@bjut.edu.cn)

Table S1. 77 RNAs in the dataset constructed by us and their PCC values obtained by the three GNM methods

|  |  |  |  |
| --- | --- | --- | --- |
| PDB ID | Number of nucleotides | Description | PCC values |
| GNM | pfGNM | mGNM |
| 1D4R | 87 | 29-mer fragment of human srp RNA helix 6 | 0.132  | 0.069  | 0.814  |
| 1DDY | 140 | Molecular recognition by the vitamin b12 RNA aptamer | 0.639  | 0.668  | 0.715  |
| 1DUQ | 104 | rev binding element of HIV-1 | 0.187  | 0.016  | 0.642  |
| 1KXK | 70 | RNA molecule containing domain 5 and 6 of the yeast ai5g group ii self-splicing intron | 0.221  | -0.208  | 0.798  |
| 1NUJ | 96 | The leadzyme structure | 0.184  | 0.104  | 0.546  |
| 1Q93 | 81 | mutant of the sarcin/ricin domain from rat 28S rRNA | 0.551  | -0.057  | 0.733  |
| 1QBP | 90 | brominated RNA helix with four mismatched base pairs | 0.707  | 0.210  | 0.731  |
| 1T0D | 66 | 2-aminopurine labelled bacterial decoding site RNA | 0.184  | 0.134  | 0.646  |
| 1U9S | 161 | specificity domain of ribonuclease P of the A-type | 0.585  | 0.433  | 0.696  |
| 1VTQ | 75 | yeast tRNAasp | 0.952  | -0.046  | 0.998  |
| 1Y26 | 71 | A-riboswitch | 0.721  | 0.608  | 0.756  |
| 1Y27 | 68 | G-riboswitch | 0.236  | -0.195  | 0.813  |
| 1YLS | 98 | selenium-modified Diels-Alder ribozyme complexed with the product of the reaction between N-pentylmaleimide and covalently attached 9-hydroxymethylanthracene | 0.206  | 0.046  | 0.557  |
| 1Z43 | 101 | 7S.S SRP RNA of M. jannaschii | 0.354  | -0.070  | 0.689  |
| 1ZX7 | 116 | Molecular recognition | 0.260  | 0.199  | 0.589  |
| 2CKY | 154 | Arabidopsis thaliana thiamine pyrophosphate riboswitch with its regulatory ligand | 0.471  | 0.334  | 0.632  |
| 2GCS | 152 | thermoanaerobacter tengcongensis glmS ribozyme | 0.825  | 0.700  | 0.816  |
| 2GDI | 160 | thiamine pyrophosphate-specific riboswitch in complex with thiamine pyrophosphate | 0.095  | -0.013  | 0.535  |
| 2GIS | 94 | S-adenosylmethionine riboswitch mRNA regulatory element | 0.457  | 0.412  | 0.733  |
| 2NOK | 88 | RNA domain from Hepatitis C virus | 0.423  | 0.384  | 0.780  |
| 2OEU | 63 | hammerhead ribozyme with Mn(II) bound | 0.257  | -0.329  | 0.689  |
| 2OIU | 142 | L1 Ribozyme Ligase circular adduct | 0.374  | 0.051  | 0.672  |
| 2QBZ | 161 | M-Box Riboswitch Aptamer Domain | 0.340  | 0.329  | 0.717  |
| 2QUS | 138 | Hammerhead Ribozyme G12A mutant pre-cleavage | 0.322  | -0.003  | 0.560  |
| 2QWY | 156 | SAM-II riboswitch bound to S-adenosylmethionine | 0.571  | 0.534  | 0.630  |
| 2TRA | 75 | yeast aspartic acid tRNA | 0.563  | 0.318  | 0.763  |
| 2YIE | 111 | F. nucleatum FMN riboswitch bound to FMN | 0.742  | 0.571  | 0.794  |
| 3BNN | 84 | homo sapiens mitochondrial ribosomal decoding site | 0.181  | 0.056  | 0.495  |
| 3BNO | 84 | homo sapiens mitochondrial ribosomal decoding site  | 0.188  | 0.112  | 0.592  |
| 3D0U | 161 | Lysine Riboswitch Bound to Lysine | 0.377  | 0.247  | 0.637  |
| 3DS7 | 134 | RNA-2'-deoxyguanosine complex | 0.664  | 0.597  | 0.690  |
| 3FU2 | 102 | class-I preQ1 riboswitch | 0.532  | 0.417  | 0.795  |
| 3IVN | 140 | U65C mutant A-riboswitch aptamer from the Bacillus subtilis pbuE operon | 0.381  | 0.151  | 0.734  |
| 3L0U | 76 | unmodified tRNAPhe from Escherichia coli | 0.261  | 0.229  | 0.834  |
| 3LA5 | 71 | mc6 RNA Riboswitch bound to azacytosine | 0.816  | 0.702  | 0.840  |
| 3OWI | 176 | the glycine riboswitch bound to glycine | 0.618  | 0.482  | 0.706  |
| 3P22 | 196 | viral RNA stability element | 0.180  | 0.075  | 0.667  |
| 3Q3Z | 150 | c-di-GMP-II riboswitch | 0.420  | 0.290  | 0.673  |
| 3RG5 | 172 | Mouse tRNA(Sec) | 0.602  | 0.458  | 0.714  |
| 3SD3 | 89 | tetrahydrofolate riboswitch containing a U25C mutation | 0.426  | 0.341  | 0.762  |
| 3SKI | 136 | 2'- Deoxyguanosine riboswitch bound to 2'-deoxyguanosine | 0.349  | 0.290  | 0.580  |
| 3SUH | 101 | THF riboswitch, bound with 5-formyl-THF | 0.898  | 0.847  | 0.901  |
| 4FRG | 168 | the cobalamin riboswitch | 0.317  | 0.317  | 0.596  |
| 4JF2 | 77 | class II preQ1 riboswitch  | 0.468  | 0.275  | 0.754  |
| 4JRC | 114 | Distal Stem I region from G. kaustophilus glyQS T box RNA | 0.848  | 0.590  | 0.886  |
| 4L81 | 96 | SAM-I/IV riboswitch  | 0.341  | 0.343  | 0.660  |
| 4P5J | 86 | tRNA-like structure  | 0.628  | 0.499  | 0.775  |
| 4P9R | 192 | group I intron  | 0.520  | 0.467  | 0.668  |
| 4PQV | 68 | Xrn1-resistant RNA  | 0.305  | 0.262  | 0.774  |
| 4QLM | 125 | ydao riboswitch binding to c-di-AMP | 0.757  | 0.700  | 0.795  |
| 4RGE | 168 | the in-line aligned env22 twister ribozyme | 0.530  | 0.398  | 0.732  |
| 4RUM | 94 | NiCo transition-metal riboswitch bound to cobalt | 0.602  | 0.393  | 0.808  |
| 4RZD | 101 | PreQ1 Riboswitch | 0.719  | 0.457  | 0.856  |
| 4TS0 | 91 | Spinach RNA aptamer | 0.699  | 0.633  | 0.769  |
| 4TZX | 71 | Vibrio Vulnificus Adenine Riboswitch variant | 0.714  | 0.655  | 0.765  |
| 4WFL | 107 | complete bacterial SRP Alu domain | 0.619  | 0.449  | 0.852  |
| 4XW7 | 64 | ZMP riboswitch | 0.175  | 0.054  | 0.688  |
| 4Y1M | 200 | Escherichia coli Mn riboswitch | 0.700  | 0.430  | 0.804  |
| 4YAZ | 168 | 3',3'-cGAMP riboswitch bound with 3',3'-cGAMP | 0.484  | 0.439  | 0.577  |
| 4ZNP | 146 | A pfI Riboswitch | 0.621  | 0.637  | 0.861  |
| 5BJO | 72 | Corn RNA aptamer | 0.598  | 0.428  | 0.790  |
| 5BTM | 110 | AUUCU repeating RNA | 0.542  | 0.219  | 0.774  |
| 5BTP | 150 | ZTP riboswitch | 0.824  | 0.734  | 0.872  |
| 5EAO | 68 | the hammerhead ribozyme | 0.238  | 0.210  | 0.645  |
| 5FJ1 | 192 | standard kink turn HmKt-7 as stem loop in P212121 space group | 0.618  | 0.499  | 0.713  |
| 5KPY | 71 | 5-hydroxytryptophan aptamer | 0.746  | 0.611  | 0.882  |
| 5KTJ | 130 | self-cleaving ribozyme | 0.324  | -0.149  | 0.788  |
| 5LYS | 114 | 7SK 5'-hairpin - Gold derivative | 0.900  | 0.738  | 0.943  |
| 5NDI | 80 | E.coli guanidine II riboswitch  | 0.210  | -0.301  | 0.502  |
| 5NWQ | 82 | thermobifida fusca guanidine III riboswitch with guanidine | 0.680  | 0.179  | 0.836  |
| 5OB3 | 69 | iSpinach aptamer | 0.841  | 0.746  | 0.909  |
| 5T3K | 66 | ribosomal decoding site | 0.258  | 0.101  | 0.671  |
| 5T83 | 95 | guanidine-I riboswitch from S. acidophilus | 0.649  | 0.631  | 0.799  |
| 5TPY | 71 | an exonuclease resistant RNA from Zika virus | 0.716  | 0.639  | 0.743  |
| 5U3G | 85 | guanidinium | 0.569  | 0.276  | 0.726  |
| 5UNE | 94 | RNA Gene: HAR1 | 0.578  | 0.515  | 0.733  |
| 6C63 | 104 | the Mango-II Fluorescent Aptamer  | 0.529  | 0.166  | 0.766  |

Table S2: The average PCC values using pfANM with different inverse powers of inter-residue distance.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| power | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| PCC | 0.321 | 0.319 | 0.318 | 0.316 | 0.311 | 0.303 | 0.294 | 0.287 | 0.282 |

1. (B) (C)



Figure S1. Crystal structures of three RNAs. (A) Fragment of helix 6 of human signal recognition particle (SRP) RNA (PDB ID: 1D4R), (B) ZMP riboswitch (PDB ID: 4XW7), and (C) G-riboswitch-guanine complex (PDB ID: 1Y27) with some main segments labeled with different colors.

Figure S2: The optimization process of parameters *η1, η2 , η3, k1 , k2 ,k3* of mGNM