User manual

RNAStat can be used to calculate structural information of RNA 3D structure(s) include four modules: (1) the radius of gyration (i.e., size) and shape; (2) the secondary structure motifs; (3) the geometry of base-pairing and base-stacking; (4) the distances between atoms;

1. Calculate the radius of gyration and shape parameter for RNA structures.

Note: PDB format, e.g., .cif

1. Calculate the size and shape of RNA structure.

run *size\_shape.exe* file ---> Enter 0 to select a single file---> Enter the path of the RNA structure, such as D:\dataset\1b7f.cif.

1. Calculate the size and shape of RNA structures.

run *size\_shape.exe* file ---> Enter 1 to select dataset---> Enter the path of the RNA structure dataset, such as D:\ dataset\---> Enter the path of results, such as

D:\ save\_path\---> output *size\_shape.csv*, meaning of document see ReadMe of the file of Statistical results.

1. Obtain the secondary structure motifs.
2. Run *cmd.exe* to call the DSSR---> Please put DSSR and RNA structures in the same folder---> Output json file, which is analyzed by DSSR(<http://x3dna.org/>)
3. Please put the JSON file in a folder (no other file), such as, D:\json\---> Run *motifs\_stat.exe* to obtain the secondary structure motifs---> Enter the json file path, such as D:\json\---> Enter the save\_file path, such as D:\ ---> Output *basepairs.csv* and *motif\_stat.csv*, meaning of document see ReadMe of the file of Statistical results.
4. Calculate the geometry of base-pairing and base-stacking.

Note: Please run *motifs\_stat.exe* to get *basepairs.csv* file first

1. run *base-pairing.exe* ---> Enter the path of dataset, such as *D:\ dataset\* ---> Enter the save\_file path, such as D:\ ---> Enter the path of *basepairs.csv--->* output base-pairing.csv, meaning of document see ReadMe of the file of Statistical results.
2. run base-stacking.exe---> Enter the path of dataset, such as *D:\ dataset\* ---> Enter the save\_file path, such as D:\ ---> Enter the path of *basepairs.csv--->* output base-pairing.csv, meaning of document see ReadMe of the file of Statistical results.
3. Calculate the distances between atoms of RNA structure(s).
4. Calculate the distance between any two atoms

Run *atom\_distance.exe* ---> Enter 1 to Calculate the distance between any two atoms ---> Enter 0 to select single file (or Enter 1 to select dataset) ---> Enter the path to store the file(.txt), such as D:/distance.txt---> Input the spacing of atomic distances(1-5), such as, 1: The distance between two atoms in the nearest neighbor nucleotides, 2 :The distance between two atoms in the second-nearest neighbor nucleotides and so on---> Enter the atoms name ---> Enter the path of RNA structure file(s), such as D:/dataset/1a9n.cif(D:/dataset/) ---> Output xx.txt, meaning of document see ReadMe of the file of Statistical results.

1. Calculate the distance between two atoms in base (A, U, G, C)

Run *atom\_distance.exe* ---> Refer to the previous step

1. Calculate the distance between atoms in different base pairs (A-U, G-C…)

Run *atom\_distance.exe* ---> Refer to the previous step