DETERMINATION OF SORT AND POSITION OF IONS IN RNA-IONS INTERACTION WITH USING EMPIRICAL POTENTIAL METHOD

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Introduction

Ions interacting with RNA molecules play a very important role in RNA folding and functioning. For example, magnesium ions stabilize the tRNA ternary structure and catalyze a reaction during ribosome assembly [1]. Thus, prediction of ion bound in new RNA structures (or in models of structures obtained *in silico*) and correction RNA conformation taking into account information on proper ion binding make important problems.

Material and Methods

We use a knowledge-based potential approach. [2] This statistical method, based on Boltzmann equation, allows one to calculate statistical preference (pseudoenergy) of ion to bound at each point near structure. According to our definitions, empirical potential is equal to a logarithm of ratio between the expected and the observed frequencies of contacts atom between structure and ion. A point with the greater pseudoenergy is the most probable site of ion binding. Essentially construction of the empirical potential is computation of the observed and the expected frequencies. The observed frequency can be evaluated by collecting of contacts between ions and atoms of RNA structure and building the histogram of distribution. In the case of the expected frequency, we use a MCRS (Monte Carlo Reference State) method, which works correctly in the case of interaction of protein with ions [3].

Magnesium, potassium, and sodium, the positively charged ions, interact with RNA phosphate backbone by electrostatic forces. Our objective was to predict preferred location of binding of these ions. For this purpose, we selected all RNA structures from PDB, which contained only one type of ion and had the pair homology less than 35%. From this set we excluded a test set, amounting to 10% from each set.

Results

We developed two programs, first for learning a model and second for predicting the ions. With the help of the first program we obtained tabulated potentials for ever type of atoms. For these potentials, we calculated a correct prediction of ion position (RMSD of this prediction are less or equal 1.5 angstrom) throughout the whole test set. The results are presented in Table 1.

PDB ID	Predicting Ion	Our RMSD	PDB ID	Predicting Ion	Our RMSD
1IK5	MG	0.92	3L0U	K	0.56
1Y3S	MG	1.28	1P79	K	0.55
1XPE	MG	1.04	1Y3S	K	0.98
2OIY	MG	1.05	2FD0	K	0.73
1FUF	MG	0.37	1L3Z	NA	1.44

Table 1.

References

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