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The guanidinium binding role in the single loop conformational dynamics and interaction between two loops of guanidine-II riboswitch

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Abstract

Riboswitches are regulatory elements in mRNA that bind specific ligands, usually leading to the stabilization of a conformation that results in a changed level of gene expression. The guanidine-II (mini-ykkC) riboswitch is the smallest of the guanidine-responsive riboswitches, comprising two stem loops of similar sequence could detect guanidinium ion leading to conformational changes at the messenger RNA level that sequester or expose regulatory sequences that control gene expression. The dimerization creates specific binding pockets for two guanidine molecules, explaining their cooperative binding. In this study, the conformational dynamics of the loop from the riboswitch was characterized in both of binding and ligand-free structures. Also, one chain and two loop stabilization were reviewed in presence of guanidinium and in absence of it and the K_d of each binding sites were obtained which was a sign of cooperativity between them.

This project was conducted in collaboration with Prof. Giovanni Bussi at the SISSA in Italy.

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