

P017 The conformational landscape of the ribosomal protein S15 and its influence on the protein interaction with 16S RNA
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The ribosomal protein S15 is among the first proteins to interact with the 16S RNA during the formation of the ribosome 30s subunit. Several crystallographic and NMR structures display conformations of the protein with different orientations of its N terminal helix $\alpha 1$. On the other hand, the presence of Mg^{2+} ions enhance the S15 binding. Biomolecular simulations of S15 and of the S15-RNA complex permitted to relate these two observations and to propose a model for the S15-RNA interaction. The recalculation of the S15 NMR structure, as well as the recording of MD trajectories, reveals that several orientations of the N-terminal helix $\alpha 1$ with respect to the structure core are populated. MD trajectories of the complex between the ribosomal protein S15 and RNA were also calculated in the presence and absence of Mg^{2+} ions. When the Mg^{2+} ions are removed, the internal mobility of the RNA and of the protein increases at the interaction interface close to the RNA G-U/G-C motif as a result of a gap between the phosphate groups in the UUCG capping tetraloop and of the disruption of S15-RNA hydrogen bonds in that region. On the other hand, several S15-RNA hydrogen bonds are reinforced, and water bridges appear between the three-way junction region and S15. The network of hydrogen bonds observed in the loop between $\alpha 1$ and $\alpha 2$ is consequently reorganized. In the absence of Mg^{2+} , this network has the same pattern as the network observed in the isolated protein, where the helix $\alpha 1$ is mobile with respect to the protein core. The presence of Mg^{2+} ions may thus play a role in stabilizing the orientation of the helix $\alpha 1$ of S15.