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Using UA-QCMD for Prediction and Characterization of RNA-Protein Complexes

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Introduction: Functional RNA's are attracting renewed attention not only in functional genome wide analysis -since they constitute a large fraction of the non-coding DNA- but in pharmaceutical related fields as well because they constitute new targets for drug development, or new therapeutic molecules per se.

Methodology: Understanding RNA interactions with proteins constitutes the first step in the analysis of their function, and several studies have been performed so far in this direction, namely using bioinformatics methodologies.

Here we combine this type of methodologies, namely RNA-Protein docking with Quantum chemical molecular dynamics (QCMD) in order to characterize the main terms driving the interaction between RNA and proteins.

Results: *Fig.1* shows the native and docking results for for tRNA-uridine uracilmutase. protein constituted of 270 amino acids and Leucyl Trna, a 70 bases long RNA. After a QCMD calculation, the results show a tendency for strong electrostatic interaction of the molecules. Further characterization of these type of complexes lead to generalization of the type of amino acids critical in RNA-protein interactions.

Fig.1 Experimental (light) and automatically predicted (dark) structure of tRNA-uridine uracil-mutase complex