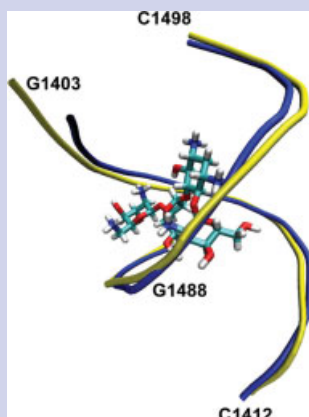


Minimizing Structure Requirements

In an article on p. 95, Anderson and Mecozzi report the use of a computational method that combines molecular dynamics simulations and free-energy calculations to predict the minimal RNA structural requirements necessary for high affinity, selective binding of small molecules.

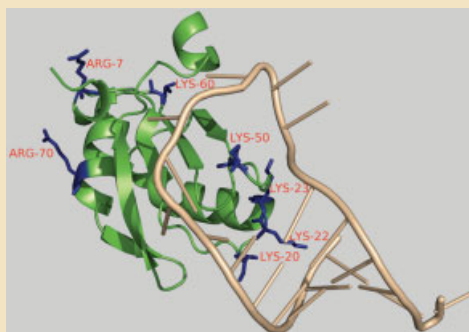
In this study, they apply their method to examine the binding of the naturally-occurring antibiotic paromomycin to a truncated bacterial 16S ribosomal RNA duplex that contains an A-site, which is targeted by paromomycin. The minimal RNA structure predicted to retain high-affinity, selective binding is verified experimentally.

Anderson, P.C. and Mecozzi, S. *Minimum Sequence Requirements for the Binding of Paromomycin to the rRNA Decoding Site A*, p. 95.



Binding Predictions

In a report on p. 112, Qin and Zhou examine how the choice of dielectric boundary can influence stability predictions based on electrostatic interaction in protein-RNA complex formation. They find that in cases where Poisson-Boltzmann calculations with the molecular (solvent exclusion) surface set as the dielectric boundary predicted positive energies from electrostatic interaction (destabilizing), using the van der Waals surface in the calculation predicts a negative (stabilizing) electrostatic interaction energy, in closer agreement with experimental data.



Qin, S. and Zhou H.-X. *Do Electrostatic Interactions Destabilize Protein-Nucleic Acid Binding?* p. 112.