Salt corrections for RNA secondary structures in the ViennaRNA package

Supplementary Data

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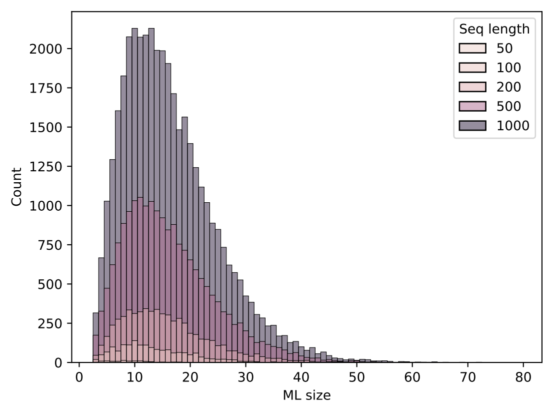


Figure S1: Length distribution of multiloops. Distribution of multiloop size L, number of backbones, among MFE structures of 5 000 uniformly selected sequences at varied length.

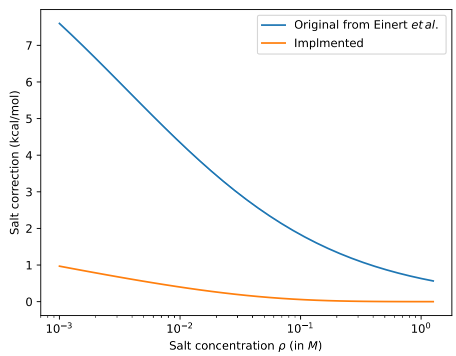


Figure S2: Approximation Error for K_0. In [1] an approximation for the difference of K_0 at a given concentration and $1M$ was proposed. However, we noticed that this approximation yields a non-vanishing salt correction at $1M$. We therefore used the Cephes library to compute K_0 directly. The panel shows the salt correction of base pair stack at $37°C$ in the function of salt concentration using the approximation (blue) and the precise computation implemented in `ViennaRNA` (orange).

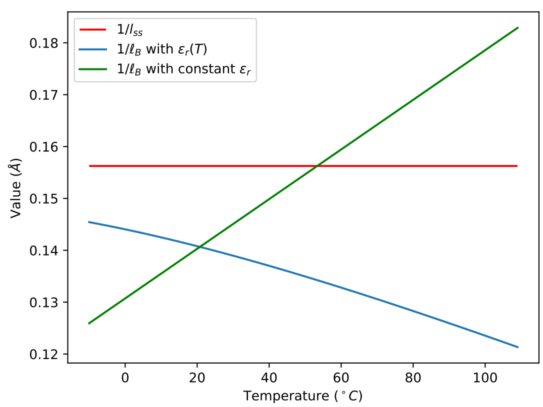
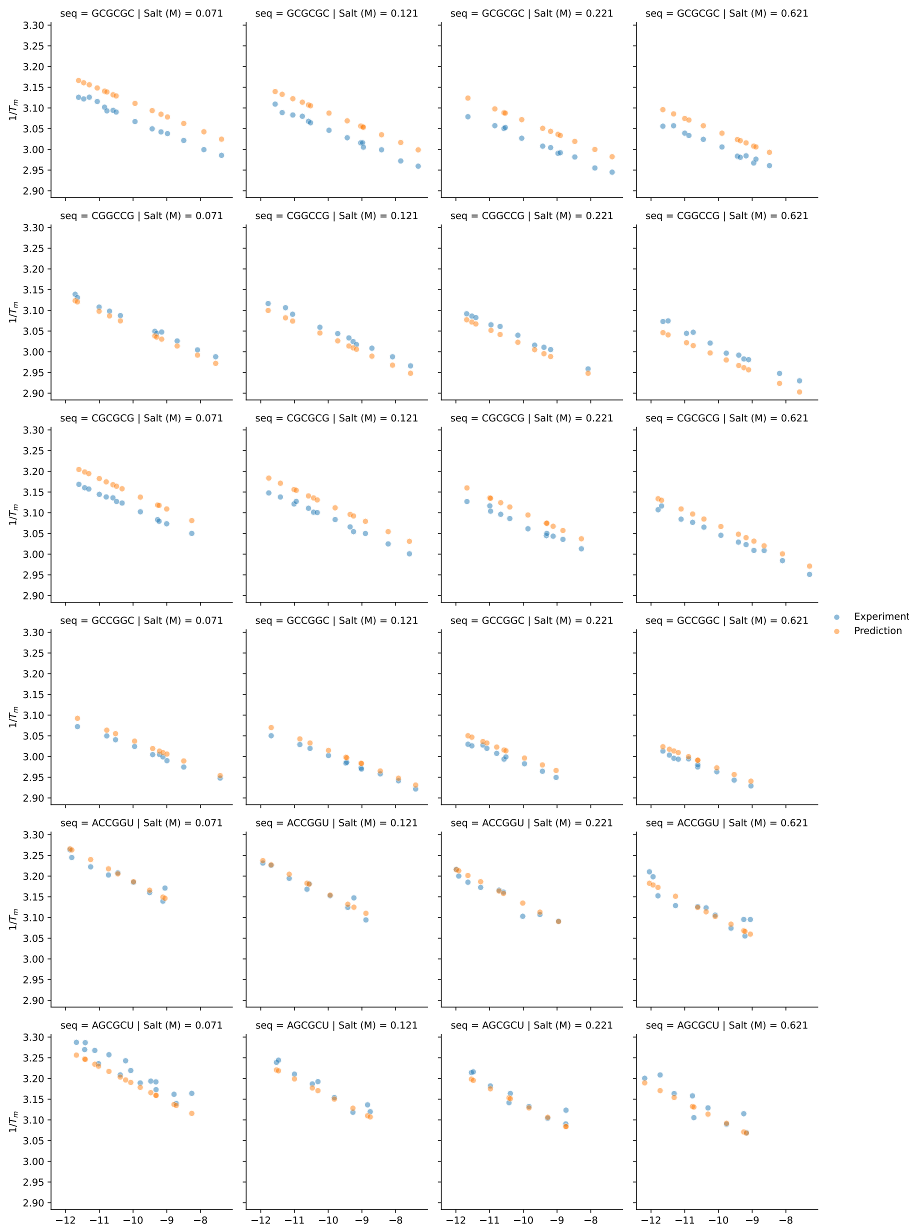


Figure S3: Nonlinear electrostatic effects τ_{ss}. In [1], the permittivity (relative dielectric constant) ϵ_r of water $\epsilon_r \approx 80$ is assumed to be temperature independent. This assumption results in a discontinuity of τ_{ss} at around $53.3\,°C$. Incorporating the empirical temperature dependence of ϵ_r results in $1/\ell_B < 1/l_{ss}$.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seq = CGGCCG | Salt (M) = 0.621
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seq = CGCGCG | Salt (M) = 0.121
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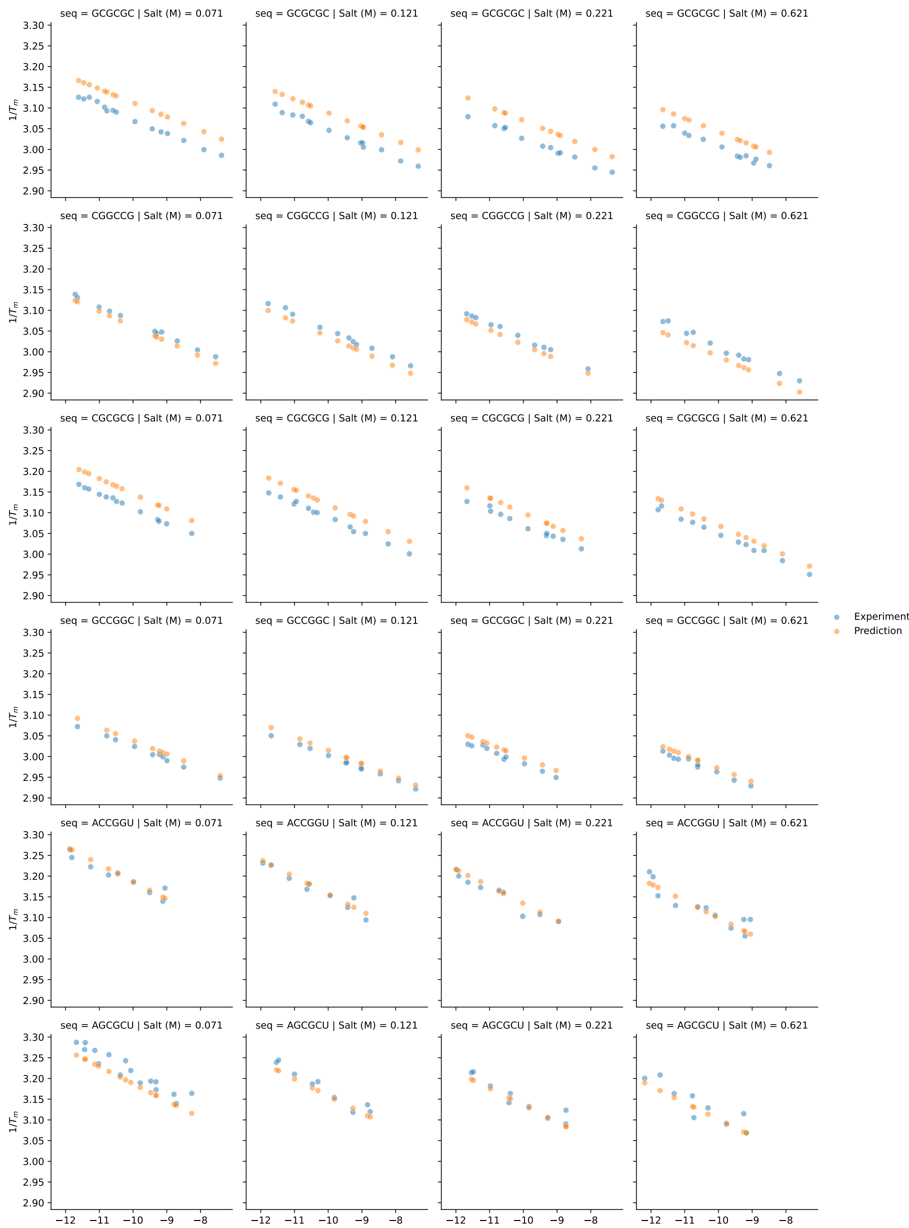
seq = AGCGCU | Salt (M) = 0.121
seq = AGCGCU | Salt (M) = 0.221
seq = AGCGCU | Salt (M) = 0.621
$1/T_m$
ln C_t
Experiment
Prediction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seq = CGGCCG | Salt (M) = 0.121
seq = CGGCCG | Salt (M) = 0.221
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seq = AGCGCU | Salt (M) = 0.621
$1/T_m$
$\ln C_t$
Experiment
Prediction

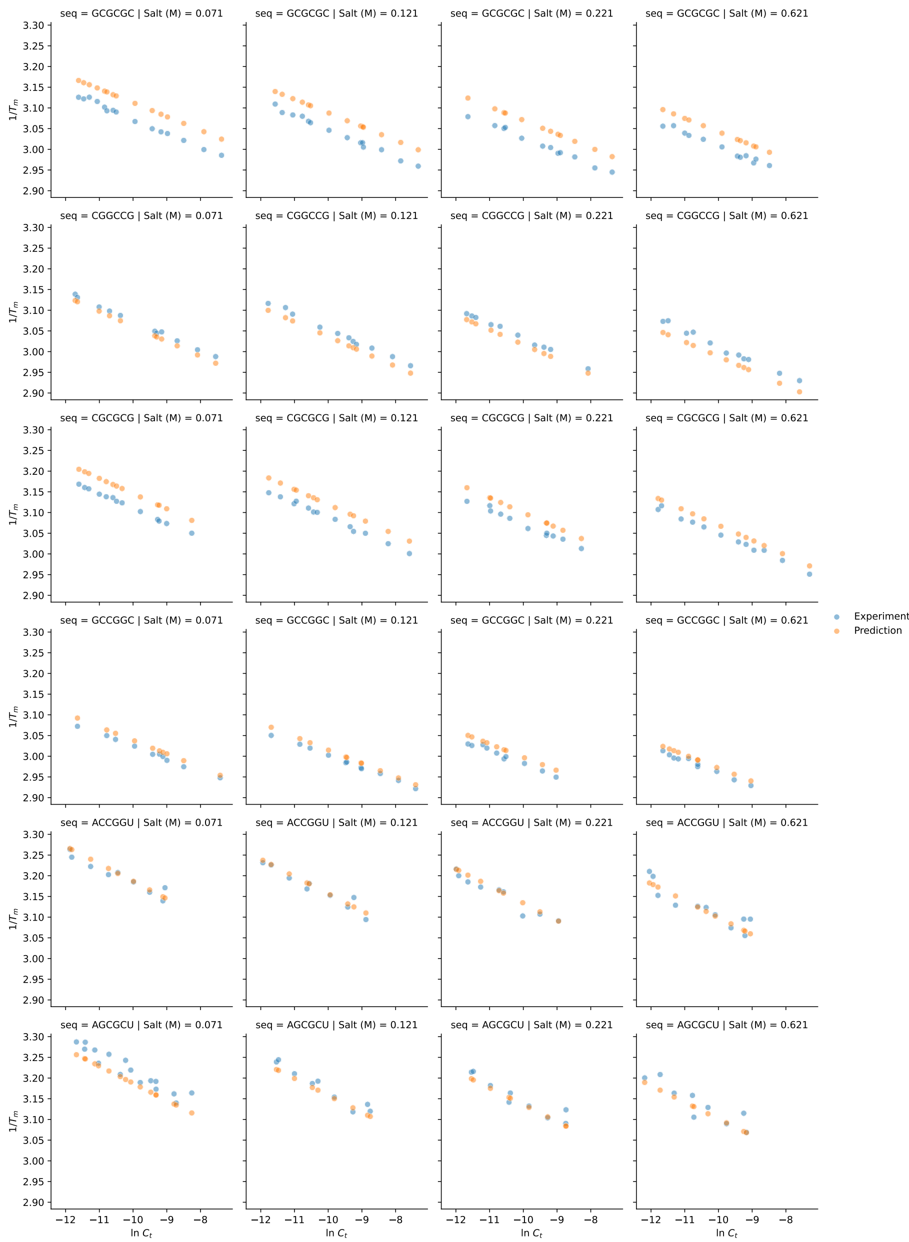

Figure S4: Van t'Hoff plots for 18 duplexes. Plotting $1/T_m$ versus $\ln c$ shows a generally good agreement of between predictions and the experimental data from from [2].

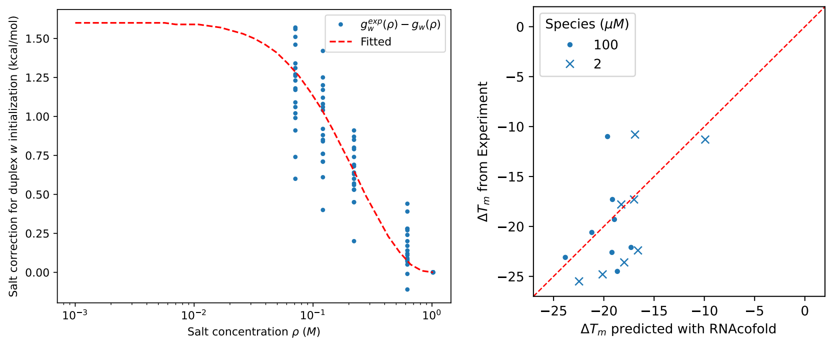

Figure S5: Converged salt correction for duplex initialization. Converged correction function fitted (left) to the difference $g_w^{\text{exp}}(\rho) - g_w(\rho)$ of 18 duplexes data [2], The plot (right) of the predicted melting temperature correction versus the experiments of longer duplexes [3] shows a better agreement with Pearson correction $r = 0.54$.

Converged salt correction for duplex initialization

$$g_{\text{init}}(\rho) = -\exp\left(a(\log(\frac{\rho}{\rho_0}))^2 + b\log(\frac{\rho}{\rho_0}) + \ln c\right) + c$$

with $a = -1.25480589$, $b = -0.05306256$, and $c = 160$. The parameter c is a constant to ensure all data points are positive in natural logarithm while fitting.

References

[1] Einert, T.R., Netz, R.R.: Theory for RNA folding, stretching, and melting including loops and salt. Biophys. J. **100**, 2745–2753 (2011). doi:10.1016/j.bpj.2011.04.038

[2] Chen, Z., Znosko, B.M.: Effect of sodium ions on RNA duplex stability. Biochemistry **52**(42), 7477–7485 (2013). doi:10.1021/bi4008275

[3] Nakano, S.-i., Kirihata, T., Fujii, S., Sakai, H., Kuwahara, M., Sawai, H., Sugimoto, N.: Influence of cationic molecules on the hairpin to duplex equilibria of self-complementary DNA and RNA oligonucleotides. Nucleic Acids Res. **35**(2), 486–494 (2007). doi:10.1093/nar/gkl1073