

NUPACK: a web-based tool for the analysis and design of nucleic acid systems

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NUPACK is a growing software suite for the analysis and design of nucleic acid systems. Current functionality includes:

- Thermodynamic analysis of dilute solutions (e.g., a test tube) of interacting nucleic acid strands in the absence of pseudoknots [1].
- Thermodynamic analysis of non-interacting strands with the possibility of certain physically-relevant pseudoknots [2, 3].
- Efficient hierarchical sequence design based on both positive and negative thermodynamic design paradigms (i.e., affinity and specificity for a target secondary structure) [4].

To enable easy access to biologists and molecular engineers worldwide, we have developed a user-friendly interactive web interface (www.nupack.org) that dramatically accelerates the rate at which hypotheses and designs can be tested computationally. Our poster will demonstrate the unique capabilities and ease of use of the NUPACK server.

References

- [1] R. M. Dirks, J. S. Bois, J. M. Schaeffer, E. Winfree, N. A. Pierce, Thermodynamic analysis of interacting nucleic acid strands, *SIAM Rev* **49**, 65–68 (2007).
- [2] R. M. Dirks, N. A. Pierce, A partition function algorithm for nucleic acid secondary structure including pseudoknots, *J Comput Chem* **24**, 1664–1677 (2003).
- [3] R. M. Dirks, N. A. Pierce, An algorithm for computing nucleic acid base-pairing probabilities including pseudoknots, *J Comput Chem* **25**, 1295–1304 (2004).
- [4] J. N. Zadeh, R. M. Dirks, N. A. Pierce, Efficient hierarchical sequence design for nucleic acid structural engineering. In preparation .