Preface

This is the second of two issues of *Biopolymers—Nucleic Acid Sciences* devoted to advances in computational modeling and molecular simulation applied to nucleic acids. As in the previous issue in this series, each of these speak in their own way to current developments important to the fields of biochemistry, structural biology and molecular biology. Filip Lankas reports on a project aimed ultimately at using molecular dynamics to derive parameters for mesoscale modeling of DNA using a sequence dependent rod model formalism based on a generalized Young's modulus tensor. Tamar Schick and coworkers report new studies of structural motifs in computational modeling related to ribosomal RNA. Steve Harvey and his group describe studies at the *meso* level related to packaging in viral capsids. Two papers, one by Dragana Djuranovich and Brigitte Hartmann and a second by Suzie Byun and I use the interesting crystallographic studies from the groups of Rashmi Hegdi and Zippora Shakked on papilloma virus DNA structures to address separate issues in the conformational and helicoidal fine structure of DNA and the comparison of structures of oligonucleotides in crystals and in solution. Finally, I have included a recent review from this laboratory on molecular dynamics simulation studies of DNA curvature and flexibility which surveys some ideas about the helix phasing problem and a new model for the pre-melting transition in DNA oligonucleotides.

While the articles included in the two issues are by necessity a selective and not totally comprehensive set, I have tried to catch the essence of new work in this field as new developments in high performance computing allow us to construct computational models that are much improved representations of the *in vitro* and *in vivo* condensed phase environment of nucleic acids. The latest detailed comparison of the performance of MD compared with experimental results obtained from NMR using residual dipolar coupling to obtain higher resolution structure (See for example Arthanari et al. *Biopolymers* 68, 3–15 (2002)) indicate that the a comparison of calculated and observed structures is quite close for the prototype case of the d(CGCGAATTCGCG) duplex. Currently emerging NMR/RDC structures on oligonucleotides, interesting of course in their own right, will also provide a valuable basis for critical testing of MD force field and simulation protocols. The issue of the convergence and stability of MD always requires careful attention in each application study. There is a potential quasi-ergodic problem lurking in the possible conformational and helicoidal substates of DNA biopolymers, and the convergence of the structures and motions of mobile counterions remains a somewhat open question. However, the currently longest simulation so far on DNA in solution, 60 nanoseconds, (see Ponomarev et al. J. Am. Chem. Soc., submitted) provides what to us is a hopeful outlook on the ion sampling problem. A key step in carrying MD to simulation to the ionic components of biological systems will also depend on the accuracy of ion potentials and possible the role of polarizability, which is currently being much discussed.

In conclusion, I would like to personally thank all the contributers to both issues, my colleague David Case for inviting me to be the guest editor for this series, and Ethan Pavlo of the Biopolymers editorial staff for his patience as the actual time scale for this project deviated by a factor of two or so from the ideal. I hope the results are worth the wait, but that's for you to decide.

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Issue Editor

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