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Journal of Molecular Graphics and Modelling 22 (2004) 317
Journal of Molecular Graphics and Modelling
www.elsevier.com/locate/JMGM

Foreword

It is with pleasure that we present to the readers this special issue of the Journal of Molecular Graphics & Modelling. There are twelve excellent articles in this issue, dealing with one of the most important problems in today's state-of-the-art simulations: conformational sampling. Traditional Sampling techniques such as Molecular dynamics (MD) and Monte Carlo (MC) suffer from the long times required to cross potential energy barriers at temperatures of interest. This is a non-trivial problem that frustrates researchers' attempts to gain new insight into complex problems through computer simulation. Enhanced sampling techniques attempt to overcome these limitations by a wide variety of methods. The present issue is meant to be a (necessarily incomplete) showcase of modern approaches to this crucial problem. The genesis of this issue can be traced to a symposium on "Enhanced Sampling Techniques in Molecular Dynamics and Monte Carlo Simulations" held within the Computers in Chemistry division of the American Chemical Society, in their 223rd annual meeting. These sessions where conducted in Orlando, FL, in April 2002. Through discussions held at that meeting, we recognized the benefit of simultaneously presenting alternative and clever approaches to the sampling problem, and we thus obtained detailed reports of the research and organized them for readers in a single volume of this well regarded publication. We wish to extend our gratitude to the authors of the articles, to Prof. Ralph Wheeler for suggesting that we organize the original sessions, and to Prof. Jonathan Essex who was instrumental in helping us create this issue for JMGM. We also gratefully acknowledge support obtained through the American Chemical Society's Petroleum Research Fund, for partial support of the meeting in Orlando through grant 37802-SE. We hope that you enjoy reading and learning from these articles as much as we did while preparing this special issue.

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1093-3263/$ – see front matter
doi:10.1016/j.jmgm.2004.03.015