American Chemical Society
Division of Computers in Chemistry
236th ACS National Meeting, Philadelphia, PA, August 17-21, 2008

J. D. Madura, Program Chair; E. X. Esposito, Program Chair; A. Roitberg, Program Chair

SUNDAY MORNING

Molecular Mechanics
E. X. Esposito, Organizer; D. R. Roe, Presiding Papers 1-7

Quantum Chemistry
A. Roitberg, Organizer; M. Mandziuk, Presiding Papers 8-13

Free Energy Simulation: From Academic Research to Industrial Application
W. Yang, Organizer Papers 14-19

Computational Approaches for Fragment Screening
D. Joseph-McCarthy, Organizer Papers 20-26

Pharmacology: The Forgotten Art of Drug Discovery
T. I. Oprea, Organizer Papers 27-34

SUNDAY AFTERNOON

Molecular Mechanics Force Field Development
Y. Duan, Organizer Papers 35-39

Challenges in Computational Chemistry
A. Nicholls, Organizer Papers 40-45

Targeting Protein Kinases in Drug Design
E. Lunney, Organizer Papers 46-49

Molecular Mechanics
E. X. Esposito, Organizer; M. R. Landon, Presiding Papers 50-55

Emerging Technologies
C. M. Breneman, Organizer Papers 56-62

MONDAY MORNING

Molecular Mechanics
E. X. Esposito, Organizer; V. Chandrasekaran, Presiding Papers 63-68

Quantum Chemistry
A. Roitberg, Organizer; D. J. Sindhikara, Presiding Papers 69-74

Free Energy Simulation: From Academic Research to Industrial Application
W. Yang, Organizer Papers 75-79

Computational Approaches for Fragment Screening
D. Joseph-McCarthy, Organizer Papers 80-86

Pharmacology: The Forgotten Art of Drug Discovery
T. I. Oprea, Organizer Papers 87-91

MONDAY AFTERNOON

Molecular Mechanics Force Field Development
Y. Duan, Organizer Papers 92-96

Challenges in Computational Chemistry
A. Nicholls, Organizer Papers 97-102

Targeting Protein Kinases in Drug Design
E. Lunney, Organizer Papers 103-107

Molecular Mechanics
E. X. Esposito, Organizer; S. E. Nichols, Presiding Papers 108-113

Free Energy Simulation: From Academic Research to Industrial Application
W. Yang, Organizer Papers 114-119

MONDAY EVENING

Sci-Mix
E. X. Esposito, Organizer Papers 180, 186, 190, 197, 202, 226-227, 233, 240, 252, 255, 261

TUESDAY MORNING

Molecular Mechanics
E. X. Esposito, Organizer; C. Bergonzo, Presiding Papers 120-126

Combining Computational Chemistry with Sequence-Based Bioinformatics for Structure-Function-Activity Relationships
T. Wymore, Organizer Papers 356-361

THURSDAY AFTERNOON

Molecular Mechanics Force Field Development
Y. Duan, Organizer Papers 362-366

Challenges in Computational Chemistry
A. Nicholls, Organizer Papers 367-372

Targeting Protein Kinases in Drug Design
E. Lunney, Organizer Papers 373-378

Exploring Chemical Reactions on Multiple Time and Length Scales with QM/MM Methods
S. T. Brown, Organizer, Presiding; A. Kohlmeyer, Organizer Papers 379-388