American Chemical Society
Division of Computers in Chemistry
235th ACS National Meeting, New Orleans, LA, April 6-10, 2008

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

SUNDAY MORNING

Computational Phase Equilibria
J. I. Siepmann, Organizer Papers 1-6

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems
S. Rick, Organizer Papers 7-11

Drug Discovery
I. Visiers, Organizer; A. Tebben, Presiding Papers 12-19

Quantum Chemistry
A. Roitberg, Organizer; J. A. Plumley, Presiding Papers 20-26

SUNDAY AFTERNOON

Computational Catalysis
A. M. Rappe, Organizer Papers 27-31

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems
S. Rick, Organizer Papers 32-36

Molecular Mechanics
E. X. Esposito, Organizer; A. J. Campbell, Presiding Papers 37-41

MONDAY MORNING

Computational Phase Equilibria
J. I. Siepmann, Organizer Papers 42-47

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems
S. Rick, Organizer Papers 48-53

Drug Discovery
I. Visiers, Organizer; J. Woolfrey, Presiding Papers 54-61

Quantum Chemistry
A. Roitberg, Organizer; C. Bergonzo, Presiding Papers 62-67

MONDAY AFTERNOON

Computational Catalysis
A. M. Rappe, Organizer Papers 68-72

Thomas Kuhn Paradigm Shift Award Competition
A. Nicholls, Organizer Papers 73-76

Quantum Chemistry
A. Roitberg, Organizer; D. J. Sindhikara, Presiding Papers 77-81

MONDAY EVENING

Sci-Mix
E. X. Esposito, Organizer Papers 116, 121, 127, 132, 136, 141, 143-144, 147, 154, 156, 162, 197, 202

TUESDAY MORNING

Computational Phase Equilibria
J. I. Siepmann, Organizer Papers 82-88

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems
S. Rick, Organizer Papers 89-92

Drug Discovery
I. Visiers, Organizer; E. Feyfant, Presiding Papers 93-98

TUESDAY AFTERNOON

Computational Catalysis
A. M. Rappe, Organizer Papers 99-104

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of J. Andrew McCammon
J. D. Madura, Organizer Papers 105-109

Molecular Mechanics
E. X. Esposito, Organizer; E. Asciutto, Presiding Papers 110-115

TUESDAY EVENING

Poster Session
E. X. Esposito, Organizer Papers 116-202

Chemical Computing Group Excellence Award
A. Good, Organizer Papers 203-207

HP Scholar Award Poster Session
C. M. Breneman, Organizer Papers 208-211

WEDNESDAY MORNING

Computational Evaluation of Rate Constants
T. N. Truong, Organizer Papers 212-217

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems
S. Rick, Organizer Papers 218-223

Drug Discovery
I. Visiers, Organizer; P. Carlqvist, Presiding Papers 224-228

WEDNESDAY AFTERNOON

Computational Catalysis
A. M. Rappe, Organizer Papers 229-234

Model Applicability Domains: When Can I Use my Model?
C. M. Breneman, Organizer Papers 235-240

Molecular Mechanics
E. X. Esposito, Organizer; C. R. Crecca, Presiding Papers 241-245

THURSDAY MORNING

Computational Evaluation of Rate Constants
T. N. Truong, Organizer Papers 246-251

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems
S. Rick, Organizer Papers 252-256

Quantum Chemistry
A. Roitberg, Organizer; V. S. Pakkala, Presiding Papers 257-262

THURSDAY AFTERNOON

Molecular Modeling Applied on DPP-4 Inhibitor Programs
Y -D. Gao, Presiding Papers 263-267

Model Applicability Domains: When Can I Use my Model?
C. M. Breneman, Organizer Papers 268-273

Molecular Mechanics
E. X. Esposito, Organizer; L. Wickstrom, Presiding Papers 274-278