

American Chemical Society
Division of Computers in Chemistry
238th ACS National Meeting, Washington, DC, August 16-20, 2009

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

SUNDAY MORNING

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 1-7

Structure Activity Relationship Knowledgebases

E. Bolton, Organizer, Presiding Papers 8-12

Quantum Chemistry

A. E. Roitberg, Organizer; J. R. Hammond, Presiding Papers 13-19

The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry

A. M. Ferreira, Organizer, Presiding Papers 20-22

Computational Chemistry in the Discovery & Development of Novel Anti-Infective Agents

G. S. Weston, Organizer, Presiding Papers 23-29

SUNDAY AFTERNOON

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 30-36

Structure Activity Relationship Knowledgebases

E. Bolton, Organizer, Presiding Papers 37-40

Molecular Mechanics

E. X. Esposito, Organizer; S. E. Nichols, Presiding Papers 41-46

Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches

H. Heinz, Organizer, Presiding Papers 47-52

Computational Chemistry in the Discovery & Development of Novel Anti-Infective Agents

G. S. Weston, Organizer, Presiding Papers 53-59

MONDAY MORNING

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 60-66

Structure Activity Relationship Knowledgebases

E. Bolton, Organizer, Presiding Papers 67-70

Quantum Chemistry

A. E. Roitberg, Organizer; F. Ding, Presiding Papers 71-76

The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry

A. M. Ferreira, Organizer, Presiding Papers 77-81

Scripting & Programming

E. X. Esposito, Organizer, Presiding; J. M. Leonard, Organizer Papers 82-86

MONDAY AFTERNOON

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 87-93

Drug Discovery

I. Visiers, Organizer, Presiding Papers 94-100

Molecular Mechanics

E. X. Esposito, Organizer; X. Cang, Presiding Papers 101-106

Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches

H. Heinz, Organizer, Presiding Papers 107-114

Emerging Technologies

C. M. Breneman, Organizer, Presiding Papers 115-121

MONDAY EVENING

Leaving the Nest: Life After Post-Doc'ing

L. M. Balbes, Organizer Paper 122

Sci-Mix

E. X. Esposito, Organizer Papers 189, 197, 206-207, 209, 212, 214, 216, 229, 236-237

TUESDAY MORNING

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 123-129

Drug Discovery

I. Visiers, Organizer, Presiding Papers 130-135

Quantum Chemistry

A. E. Roitberg, Organizer; S. Pakkala, Presiding Papers 136-140

The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry

A. M. Ferreira, Organizer, Presiding Papers 141-145

Molecular Visualization

R. E. Amaro, Organizer, Presiding Papers 146-152

TUESDAY AFTERNOON

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 153-159

Drug Discovery

I. Visiers, Organizer; J. H. Voigt, Presiding Papers 160-166

Molecular Mechanics

E. X. Esposito, Organizer; K. Shahrokh, Presiding Papers 167-172

Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches

H. Heinz, Organizer, Presiding Papers 173-178

TUESDAY EVENING

Chemical Computing Group Excellence Award

C. L. Simmerling, Organizer Papers 179-183

Hewlett-Packard Scholar Awards

C. L. Simmerling, Organizer Papers 184-187

Poster Session

E. X. Esposito, Organizer Papers 188-275

WEDNESDAY MORNING

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 276-282

Drug Discovery

I. Visiers, Organizer, Presiding Papers 283-289

Quantum Chemistry

A. E. Roitberg, Organizer; S. Manepalli, Presiding Papers 290-294

The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry

A. M. Ferreira, Organizer, Presiding Papers 295-297

Molecular Visualization

R. E. Amaro, Organizer, Presiding Papers 298-302

WEDNESDAY AFTERNOON

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 303-309

Drug Discovery

I. Visiers, Organizer; M. R. Landon, Presiding Papers 310-316

Molecular Mechanics

E. X. Esposito, Organizer; R. E. Amaro, Presiding Papers 317-321

Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches

H. Heinz, Organizer, Presiding Papers 322-327

THURSDAY MORNING

Protein Dynamics and Function

H -X. Zhou, Organizer, Presiding Papers 328-334

Drug Discovery

I. Visiers, Organizer; Y. J. Tseng, Presiding Papers 335-340

Quantum Chemistry

A. E. Roitberg, Organizer; D. R. Roe, Presiding Papers 341-346

Molecular Mechanics

E. X. Esposito, Organizer; C. Bergonzo, Presiding Papers 347-352