

American Chemical Society
Division of Computers in Chemistry
239th ACS National Meeting & Exposition, San Francisco, CA, March 21-25, 2010

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

SUNDAY MORNING

Advances in Conformational Sampling

D. Agrafiotis, Organizer; P. Liu, Organizer. Papers 1-7

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer, Presiding. Papers 8-14

Quantum Chemistry

E. X. Esposito, Organizer. Papers 15-20

Generalized-Ensemble Simulation Methods: Symposium in Honor of Dr. Bernd Berg's 60th Birthday

J. Ma, Organizer; W. Yang, Organizer; U.H.E. Hansmann, Organizer, Presiding. Papers 21-26

Molecular Mechanics

E. X. Esposito, Organizer; C. Mayne, Presiding. Papers 27-33

SUNDAY AFTERNOON

Advances in Conformational Sampling

D. Agrafiotis, Organizer; P. Liu, Organizer. Papers 34-39

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; H. Carlson, Presiding. Papers 40-45

Quantum Chemistry

E. X. Esposito, Organizer. Papers 46-51

Generalized-Ensemble Simulation Methods: Symposium in Honor of Dr. Bernd Berg's 60th Birthday

U.H.E. Hansmann, Organizer; J. Ma, Organizer; W. Yang, Organizer, Presiding. Papers 52-58

Molecular Mechanics

E. X. Esposito, Organizer; A. Carr, Presiding. Papers 59-65

Thomas Kuhn Paradigm Shift Award Symposium

A. Nicholls, Organizer; G. Skillman, Presiding. Papers 66-70

MONDAY MORNING

Advances in Conformational Sampling

D. Agrafiotis, Organizer; P. Liu, Organizer. Papers 71-77

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; S. Nichols, Presiding. Papers 78-84

Quantum Chemistry

E. X. Esposito, Organizer, Presiding. Papers 85-90

Generalized-Ensemble Simulation Methods: Symposium in Honor of Dr. Bernd Berg's 60th Birthday

U.H.E. Hansmann, Organizer; W. Yang, Organizer; J. Ma, Organizer, Presiding. Papers 91-96

Recent Advances in Computational Methods

C. Lemmen, Organizer; S.-Y. Liu, Organizer; S. Varma, Organizer; A. Nicholls, Organizer, Presiding; E. Sourial, Organizer, Presiding. Papers 97-97

MONDAY AFTERNOON

Advances in Conformational Sampling

D. Agrafiotis, Organizer; P. Liu, Organizer. Papers 98-103

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; Z. Yang, Presiding. Papers 104-109

Quantum Chemistry

E. X. Esposito, Organizer; F. Ding, Presiding. Papers 110-116

Generalized-Ensemble Simulation Methods: Symposium in Honor of Dr. Bernd Berg's 60th Birthday

U.H.E. Hansmann, Organizer; J. Ma, Organizer; W. Yang, Organizer; R. Zhou, Presiding. Papers 117-122

Recent Advances in Computational Methods

C. Lemmen, Organizer; S.-Y. Liu, Organizer; S. Varma, Organizer; A. Nicholls, Organizer, Presiding; E. Sourial, Organizer, Presiding. Papers 123-123

MONDAY EVENING

Sci-Mix

E. X. Esposito, Organizer. Papers 193-194, 198, 212, 215, 230, 235, 238, 244, 257, 267, 270, 277-278, 286, 289, 301-302, 306, 309

TUESDAY MORNING

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of Kenneth M. Merz, Jr.

A. Roitberg, Organizer, Presiding. Papers 124-128

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; J. Shen, Presiding. Papers 129-134

Quantum Chemistry

E. X. Esposito, Organizer; L. Achenie, Presiding. Papers 135-140

Generalized-Ensemble Simulation Methods: Symposium in Honor of Dr. Bernd Berg's 60th Birthday

U.H.E. Hansmann, Organizer; J. Ma, Organizer; W. Yang, Organizer; Y. Okamoto, Presiding. Papers 141-146

Recent Advances in Computational Methods

C. Lemmen, Organizer; S.-Y. Liu, Organizer; E. sourial, Organizer; S. Varma, Organizer; A. Nicholls, Organizer, Presiding. Papers 147-147

TUESDAY AFTERNOON

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of Kenneth M. Merz, Jr.

A. Roitberg, Organizer, Presiding. Papers 148-152

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; E. Sherer, Presiding. Papers 153-159

Quantum Chemistry

E. X. Esposito, Organizer; R. Swift, Presiding. Papers 160-166

Molecular Mechanics

E. X. Esposito, Organizer; J. Hsieh, Presiding. Papers 167-174

Recent Advances in Computational Methods

C. Lemmen, Organizer; S.-Y. Liu, Organizer; A. Nicholls, Organizer; S. Varma, Organizer; E. sourial, Organizer, Presiding. Papers 175-175

TUESDAY EVENING

Chemical Computing Group Excellence Award

C. Simmerling, Organizer. Papers 176-180

Hewlett-Packard Scholar Awards

C. Simmerling, Organizer. Papers 181-184

Poster Session

E. X. Esposito, Organizer. Papers 185-310

WEDNESDAY MORNING

**ACS Award for Computers in Chemical and Pharmaceutical Research:
Symposium in Honor of Kenneth M. Merz, Jr.**

A. Roitberg, Organizer, Presiding. Papers 311-316

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; I. Thorpe, Presiding. Papers 317-323

Quantum Chemistry

E. X. Esposito, Organizer. Papers 324-330

Molecular Mechanics

E. X. Esposito, Organizer; M. Lawrenz, Presiding. Papers 331-337

Recent Advances in Computational Methods

C. Lemmen, Organizer; S.-Y. Liu, Organizer; S. Varma, Organizer; A. Nicholls, Organizer, Presiding; E. sourial, Organizer, Presiding. Papers 338-338

WEDNESDAY AFTERNOON

**ACS Award for Computers in Chemical and Pharmaceutical Research:
Symposium in Honor of Kenneth M. Merz, Jr.**

A. Roitberg, Organizer, Presiding. Papers 339-343

Drug Discovery

S. Wildman, Organizer; Y.J. Tseng, Organizer, Presiding. Papers 344-349

Quantum Chemistry

E. X. Esposito, Organizer; O. Demir, Presiding. Papers 350-357

Molecular Mechanics

E. X. Esposito, Organizer. Papers 358-365

Recent Advances in Computational Methods

C. Lemmen, Organizer; S.-Y. Liu, Organizer; S. Varma, Organizer; A. Nicholls, Organizer, Presiding; E. sourial, Organizer, Presiding. Papers 366-366

THURSDAY MORNING

Molecular Mechanics

E. X. Esposito, Organizer; P. Mukherjee, Presiding. Papers 367-374

Drug Discovery

Y.J. Tseng, Organizer; S. Wildman, Organizer; R. Baron, Presiding. Papers 375-380

Quantum Chemistry

E. X. Esposito, Organizer. Papers 381-386