

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

**Quantum Chemistry**

A. Roitberg, Organizer; F. Ding, Presiding Papers 127-131

**Free Energy Simulation: From Academic Research to Industrial Application**

W. Yang, Organizer Papers 132-137

**Computational Approaches for Fragment Screening**

D. Joseph-McCarthy, Organizer Papers 138-143

**Drug Discovery**

I. Visiers, Organizer; M. Wu, Presiding Papers 144-152

## TUESDAY AFTERNOON

**Molecular Mechanics Force Field Development**

Y. Duan, Organizer Papers 153-156

**Challenges in Computational Chemistry**

A. Nicholls, Organizer Papers 157-162

**Targeting Protein Kinases in Drug Design**

E. Lunney, Organizer Papers 163-167

**Quantum Chemistry**

A. Roitberg, Organizer; Y. Meng, Presiding Papers 168-173

## TUESDAY EVENING

**Poster Session**

E. X. Esposito, Organizer Papers 174-267

**Chemical Computing Group Excellence Award**

C. L. Simmerling, Organizer Papers 268-272

**Hewlett-Packard Scholar Awards**

C. M. Breneman, Organizer Papers 273-276

## WEDNESDAY MORNING

**Molecular Mechanics**

E. X. Esposito, Organizer; R. Abel, Presiding Papers 277-283

### **Quantum Chemistry**

A. Roitberg, Organizer; S. Manepalli, Presiding Papers 284-288

### **Free Energy Simulation: From Academic Research to Industrial Application**

W. Yang, Organizer Papers 289-294

### **Combining Computational Chemistry with Sequence-Based Bioinformatics for Structure-Function-Activity Relationships**

T. Wymore, Organizer Papers 295-299

### **Drug Discovery**

I. Visiers, Organizer; E. Sherer, Presiding Papers 300-307

## WEDNESDAY AFTERNOON

### **Molecular Mechanics Force Field Development**

Y. Duan, Organizer Papers 308-311

### **Challenges in Computational Chemistry**

A. Nicholls, Organizer Papers 312-317

### **Targeting Protein Kinases in Drug Design**

E. Lunney, Organizer Papers 318-322

### **Free Energy Simulation: From Academic Research to Industrial Application**

W. Yang, Organizer Papers 323-329

### **Exploring Chemical Reactions on Multiple Time and Length Scales with QM/MM Methods**

A. Kohlmeyer, Organizer, Presiding; S. T. Brown, Organizer Papers 330-339

## THURSDAY MORNING

### **Molecular Mechanics**

E. X. Esposito, Organizer; R. J. Doerksen, Presiding Papers 340-344

### **Quantum Chemistry**

A. Roitberg, Organizer; E. K. Ascutto, Presiding Papers 345-350

### **Free Energy Simulation: From Academic Research to Industrial Application**

W. Yang, Organizer Papers 351-355

**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