The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram.
TECHNICAL PROGRAM

WEDNESDAY MORNING

Section A
Salt Palace Convention Center 254 A

Adaptive Scoring Functions Cosponsored by the CSA Trust and COMP

D. K. Agrafiotis and E. J. Martin, Organizers

Introductory Remarks.
2:00 51. Force field based scoring of protein-ligand binding affinities. J. Aqvist
3:00 53. Learning scoring function parameters from binary data. M. H. Seifert
3:50 Interm. 2:00 454. 2-D and 3-D adaptive scoring functions for iterative kinase medium-throughput put screening (MTS) with Profile-QSAR and AutoSimm. E. J. Martin, D. C. Sullivan, P. Mukherjee
4:40 55. Combining quantitative data and qualitative knowledge to score reaction energies. C. A. Azencott, M. A. Kalyali, P. Baldi

Section B
Salt Palace Convention Center 251 F

Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen

Crystal Form Analysis, Experiment and Prediction Cosponsored by COMP, CHAL, and MEDI

B. Town and F. H. Allen, Organizers

2:00 56. Drug development and solid form selection: Multicomponent crystals. W. Jones
2:30 57. Supramolecular heterosystems and their role in crystalline design. M. Zaworotko, M. L. Cheney, D. Waynita
3:00 58. Cambridge Structural Database: analysis of complementary molecular properties in co-crystals. L. Fabian
4:00 50. Pharmaceutical crystal forms at the dynamic intersection of science and intellectual property law. B. B. Masek, K. M. Smith, S. C. Nagy, J. R. Damewood, C. L. Lerman
4:30 40. Concluding Remarks.

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Section B
Salt Palace Convention Center 251 F

General Papers

R. Guha, Organizer

2:00  Introductory Remarks.
2:05 74. Text mining for chemistry and building a public platform for document markup. A. J. Williams
2:30 75. Extending the scope of journal articles: Certifying and publishing experimental data. I. S. Brase, S. Haak, G. F. Hermann
2:55 76. Ontologies for nanotechnology. C. R. Batcheller
3:20 Interm.
3:55 78. Cleaning up chemistry for the pharma industry: Delivering a flexible platform for interrogating the FDA Dai-Med website. A. Williams, P. Potenza
4:20 79. The use of EPA software and Scarton University green chemistry web page in the green engineering course in Universidad de los Andes. G. Camargo, F. Segura, A. Altamir, J. E. Tinano

THURSDAY MORNING

Section A
Salt Palace Convention Center 254 A

General Papers

R. Guha, Organizer

8:30  Introductory Remarks.
9:00 81. Development of test systems for pharmacophore elucidation. J. C. Cole, E. J. Gardner, V. J. Gillet, R. Taylor
9:50 Interm.
10:30 84. Reaction simulation system for synthetic organic chemistry. J. H. Chen, F. Bald
10:55 F. A BLAST-like tool for chemoinformatics and drug discovery. F. Bald
11:20 86. Binding of alkaloid metal cations (Li+, Na+ and K+) with mono- and bi-cyclic ring fused benazoles: A theoretical study. T. C. Dinhayalane, J. Leszczynski

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Division of Chemical Technicians

K. Hayasip, Program Chair

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