



## North American Science Summit

*Analyze, Optimize, Socialize*  
*January 28-29, 2010*

### Thursday (Day 1)

9:30 am Registration and Continental Breakfast

10:00 am Opening and welcome, Certara Vision – Patrick Flanagan

### Considering all the parameters

10:45 am Efficient and Effective Navigation of Multiparameter Design Performance  
*Jim Damewood, AstraZeneca*

11:15 am Recent Advances in Multi-criteria Drug Design  
*Brian Masek, Tripos*

12:00 pm Lunch, networking, demos

1:30 pm Identifying Novel Anthrax Toxin Lethal Factor (LF) Inhibitors Using Topomeric Searching, Docking and Scoring, Drug-Like Filtering, and In Vitro Screening  
*Ting-Lan Chiu, University of Minnesota*

### Can the experimental data be trusted?

2:30 pm An Objective View Of Ligands In The PDB: Taking Responsibility: Considering The Error In Our Data  
*Terry Stouch, TerryRichardStouch Consulting*

3:00 pm QSAR models for predicting the similarity in binding profiles for pairs of protein kinases-when datasets disagree  
*Robert P. Sheridan, Merck Research Laboratories*

3:30 pm Break, demos, networking

### Panel Discussion

4:00 pm How Drug Discovery is Changing for the Future

- How modeling needs to adapt
  - Virtual organizations
  - Smaller organizations
  - Hosted solutions

6:00 pm Evening event

## Friday (Day 2)

9:30 am Registration and continental breakfast

### Ligand Preparation and Beyond

10:00 am Tautomers: The Almost Forgotten Issue  
*Dr. Yvonne C. Martin, Martin Consulting*

10:30 am Discussion: Addressing the concepts of Chemical Structure vs. Chemical Compound in CADD  
*Brian Masek, Tripos*

11:00 am Computer-Aided Drug Design Despite Inadequate Physicochemical Models  
*Richard D. Cramer, Tripos*

11:30 am Lunch, networking, demos

1:00 pm Data Access, Analysis, and Collaboration  
*David Lewis, Tripos*

1:45 pm Computational Chemistry Workflows – Future Directions for SYBYL-X  
*Richard D. Cramer, David Lewis*

2:30 pm Break

3:00 pm Lead Optimization Challenge Results  
*Richard D. Cramer, Tripos*

4:00 pm Meeting closes