



The Institute  
of  
Chemistry of Ireland



NUI Galway  
OÉ Gaillimh

Scientific Programme, ICI Annual Conference

## High Performance Computing at the Chemistry/Biochemistry Interface

NUI Galway, May 21, 2010

09.00 - 09.30	Registration
09.30 - 09.40	Welcome
09.40 - 10.30	Bill Jorgensen, Yale <i>Efficient Drug Lead Optimization Guided by Free-Energy Calculations</i>
10.30 - 11.00	David Lloyd, TCD <i>Virtual Reality - do computational chemists dream of electronic molecules?</i>
11.00 - 11.30	Leif A. Eriksson, NUIG <i>SLC 25A43: From Gene Sequence to Protein Function.</i>
11.30 - 11.50	<b>COFFEE</b>
11.50 - 12.20	Jens Nielsen, UCD <i>Predicting the Biophysical Characteristics of Proteins: Validation Using Multiple Types of Experimental Data</i>
12.20 - 12.50	Elisa Fadda, NUIG <i>Role of surface-bound water in protein-carbohydrate recognition and binding: Concanavalin A</i>
12.50 - 14.20	<b>LUNCH + Poster Session</b>
14.20 - 15.10	Andrew R. Leach, GSK <i>tba</i>
15.10 - 15.40	Meilan Huang, QUB <i>Action Mechanism of Diketo-Acid Inhibitors for HIV-1 Integrase</i>
15.40 - 16.10	Rob Woods, NUIG <i>Predicting Influenza Species Specificity: A Case for Computational Glycoscience</i>
16.10 - 16.30	<b>COFFEE</b>
16.30 - 17.00	Damien Thompson, UCC <i>Molecular Design of Self-Assembling Materials</i>
17.00 - 17.30	Patricia Saenz Mendez, UdelaR <i>The Reaction Mechanism of Dehaloperoxidase</i>



**JANSSEN**  
PHARMACEUTICAL LTD

