

Seminar

Monday 1 August 2011

11.00 am - Room 531

Dr Jóhannes Reynisson

Senior Lecturer in Computational Chemistry & Molecular Modelling, School of Chemical Sciences,
The University of Auckland

Virtual high throughput screening in anticancer drug discovery

Using docking algorithms to generate hits and leads is now a viable alternative to the classical high throughput approach. An obvious advantage is the much lower cost of running a virtual screen. Until now I have managed three virtual screening campaigns, which all were successful in generating hit compounds. The GOLD1 software was used in conjunction with the ZINC compound collection² and the QikProp³ prediction package. As much as 30% of the acquired compounds showed activity in biochemical and cell-based assays. However, much room is left for improvement of the methodology employed and these improvements will be discussed as well as the possible pitfalls in the execution of virtual high throughput screening.

- 1 G. Jones, P. Willet, R. C. Glen, A. R. Leach, and R. Taylor, *J.Mol.Biol.*, 1997, 267, 727.
- 2 J. J. Irwin and B. K. Shoichet, *J. Chem. Inf. Model.*, 2005, 45, 177.
- 3 W. L. Jorgensen and E. M. Duffy, *Adv. Drug Del. Rev.*, 2002, 54, 355.