CERMM Technical Workshop Series

FORECASTER Computational Platform: Drug and Catalyst Design

Wednesday, December 17th, 2008. starting at 1:00PM, in room SP-S185.10, Richard J. Renaud Science Complex, Loyola Campus, Concordia University

Lecturer: Prof. Nicolas Moitessier
Department of Chemistry, McGill University

The Moitessier group has developed a computational platform (**FORECASTER**) **for molecular design**. It includes **FITTED**, **a program that docks potential drugs to biological targets** (i.e., proteins), **ACE**, **a program that predicts the stereochemical outcome of asymmetric reactions,** and **REACTOR, a program for *in silico* combinatorial chemistry and others.** The platform is available free of charge to collaborators of the Moitessier group and selected, trained, research groups.

These programs can be used on regular PCs and Linux workstations **to help chemists design efficient drugs or catalysts**. In this workshop, Nicolas Moitessier and his group members will present these programs and will describe some of the successful applications. The workshop will entail two parts: presentation of the programs and their applications in a lecture room and application of the programs using selected examples in a computer room.

For more information about the **FORECASTER** computational platform, visit http://moitessier-group.mcgill.ca/ .

SCHEDULE

1:00 – 2:30: Presentation of the FORECASTER platform and applications
2:30 – 3:00: Break
3:00 – 5:00: Practical workshop
5:00 – 7:00: Reception

Registration is free, but please register for the workshop by filling out the form on the CERMM website http://cermm-s.concordia.ca/workshops.html, or by e-mailing us at management@cermm.concordia.ca by Friday, December 12th, 2008.