Schrödinger Maestro workshop report

Schrödinger Maestro workshop was organized by CSC and Schrödinger in Espoo on 25th March 2009. It took place at the Life Science Center in Keilaniemi, Espoo. The workshop sessions were conducted by Jianxin Duan (senior applications scientist) and Annette Höglund PhD (international account and marketing manager) from Schrödinger. The lectures were given by Jianxin Duan and the hands on exercises were supervised by CSC staff and Annette Höglund. The workshop outline consisted of homology modeling and protein simulations, docking: from high throughput virtual screening to lead optimization and binding affinity predictions and ligand-based lead optimization.

The first session in the workshop started off by a lecture on protein structure prediction which focused on predicting accurate models for drug design. There was also emphasis on accuracy of loop predictions and refinement, identification and characterization of the binding sites using the SiteMap tool from Schrödinger Maestro suite. The next sessions dealt with docking and introduction to the concepts of high throughput virtual screening, affinity predictions followed by structure based pharmacophores and fragment docking using Glide Ligand Docking. The lectures were immediately followed up by hands on exercises. There was also a demonstration on how to run parallel jobs in CSC environment by submitting them to Murska cluter (at CSC). It was a bit tricky in the beginning for me and a few others who had never done this before. But we were able to get around it, our task was conformational search and it turned out it be a very fun session.

This workshop was attended by graduate students and researchers from various universities and institutes. It was a great learning experience as people discussed their project works over coffee and lunch as to how homology modeling or molecule/drug design fit in with their respective works. The people at CSC were very co-operative and offered assistance when required. I can gladly recommend this hands-on workshop for anyone interested in computer-based molecule/drug-design or homology modeling.

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