John P. McGovern Lectureship in Biomedical Computing and Imaging

On the Applicability of Molecular Models of G protein-coupled receptors to Structure-based Drug Discovery

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G protein-coupled receptors (GPCRs) are a large superfamily of membrane bound proteins involved in numerous physiological functions and pathological conditions, thus holding great pharmaceutical interest.
For several years, atomic resolution structural information has been available only for one member of the superfamily, namely bovine rhodopsin, which has been widely used as a template for the construction of homology models.
Within the last two years, the landscape of GPCR structural studies has changed significantly, with the disclosure of the X-ray structure of a number of additional members of the superfamily. As I will demonstrate, the now possible comparison of in silico models and crystal structure of a GPCR/ligand complex argues in favor of the applicability of GPCR modeling to drug discovery. I will also illustrate a number of applications of GPCR modeling to computer-assisted ligand discovery, including ligand identification through virtual screenings, ligand optimization, and the study of the activation and blockage process.

Date: Tuesday, December 2, 2008
Time: 4:30PM
Place: GSBS Large Classroom (BSRB S3.8371)
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