未来型医療創成センター／東北メディカル・メガバンク機構　主催

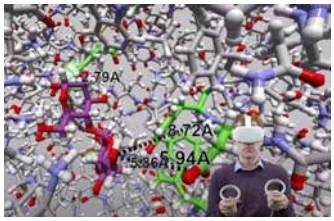
INGEM＆ToMMo セミナーシリーズ 第34回

～未来型医療の実現に向けた課題～

Interactive flexible receptor docking using DockIT

DockIT is an interactive docking tool that enables the user to dock a rigid ligand to a flexible receptor molecule. The conformational change in the receptor due to its interaction with the ligand is modelled using the method of linear response. This is achieved by first performing an explicit-solvent molecular dynamics simulation of the receptor and then performing an eigenvector decomposition of the covariance matrix of atomic displacements. This approach enables us to evaluate the conformational response in real time by: (1) exploiting a feature of protein dynamics whereby most fluctuation occurs within a relatively small subspace; (2) exploiting the power of the modern GPU to achieve maximum efficiency both in memory and computation time. DockIT also has other useful features such as real time molecular surface rendering, which presents a particular challenge in a docking tool that incorporates molecular flexibility. It also can be used in Virtual Reality using a headset and hand-held controllers. This enables particularly intuitive control as movement of the left hand is tied to the receptor and movement of the right hand is tied to the ligand.

The talk will introduce DockIT, describe some latest developments, and show results we have obtained with the cancer target protein, histone deacetylase 6, in interaction with the drug molecule belinostat.



https://dockit.uk/　※DockITについて詳しくはリンク先をご参照ください

演　者　**Professor. Steven Hayward**

School of Computing Sciences,
University of East Anglia, Norwich, UK

日　時　**2024年9月13日[金] 15:00 - 16:30**

会　場　**東北メディカル・メガバンク棟3階 大会議室**
※会場にてDockITの実演を行います
（学内向けにオンラインでも配信いたします）

事前申込不要です

お問い合わせ
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