This poster by Fayzan Ahmed, Tamsin Mansley, Chris Leeding, Edmund Champness, Peter Hunt & Matthew Segall was presented at the ACS Spring 2017 National Meeting & Exposition held in San Diego, USA.

Abstract

To prioritise new compound ideas efficiently in a discovery project, compound structures and all their associated data must be brought together to guide optimisation of high quality, potent compounds. Predictions based on 2-dimensional (2D) and 3-dimensional (3D) structures are typically generated in an arsenal of modelling tools, often restricted to expert users due to their complexity. This means that computational scientists spend time running routine calculations, distracting them from the more scientifically challenging tasks, such as preparation and validation of protein docking models, where their expertise is most valuable. The delay in feedback to the medicinal chemists also forms a barrier to rigorous assessment of new compound ideas prior to synthesis.

We will present an integrated, generic Pose Generation Interface which links expertly prepared docking and 3D alignment models, from a variety of applications, with a comprehensive environment for data visualisation, analysis and predictive modelling. Poses and scores are automatically retrieved for visualisation and analysis, alongside predictions from models of absorption, distribution, metabolism, excretion and toxicity (ADMET). This enables medicinal chemists to evaluate multiple iterations of designs on-the-fly and quickly understand structure-activity relationships, identify potential liabilities and design new compounds with the highest chance of success. While their colleagues use the 3D models they have built and validated, the computational scientists can focus on the next round of expert computational design and model building. This approach supports collaboration between computational and synthetic chemists, helping to share the results of 3D modelling studies with all decision makers.

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