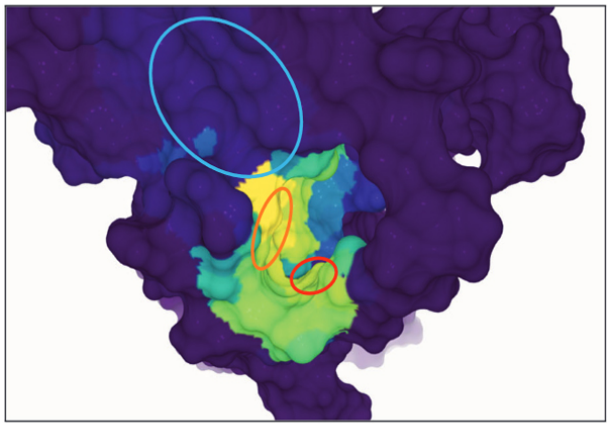
ViRVIG
Visualització, Realitat Virtual i Interacció Gràfica

www.virvig.eu
C. Llorens i Artigas 4-6
Edifici U, 1er pis
E- 08028- Barcelona

Visual Analysis of Large-Scale Protein-Ligand Interaction Data

Schatz, K.; Franco, Juan Jose; Schafer, M.; Rose, A.S.; Ferrario, V.; Pleiss, J.; Vazquez, Pere-Pau; Ertl, T.; Krone, M.



When studying protein-ligand interactions, many different factors can influence the behaviour of the protein as well as theligands. Molecular visualisation tools typically concentrate on the movement of single ligand molecules; however, viewing onlyone molecule can merely provide a hint of the overall behaviour of the system. To tackle this issue, we do not focus on thevisualisationofthelocalactionsofindividualligandmoleculesbuton theinfluenceofaproteinandtheiroverallmovement.Sincethe simulations required to study these problems can have millions of time steps, our presented system decouples visualisationand data preprocessing: our preprocessing pipeline aggregates the movement of ligand molecules relative to a receptor protein.For data analysis, we present a web-based visualisation application that combines multiple linked 2D and 3D views that displaythe previously calculated data The central view, a novel enhanced sequence diagram that shows the calculated values, is linkedto a traditional surface visualisation of the protein. This results in an interactive visualisation that is independent of the size ofthe underlying data, since the memory footprint of the aggregated data for visualisation is constant and very low, even if the rawinput consisted of several terabytes.

http://dx.doi.org/10.1111/cgf.14386

UPC