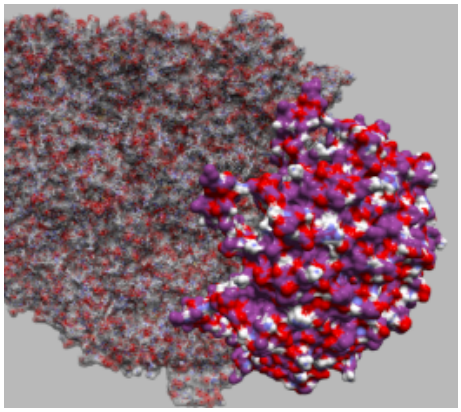
University of East Anglia

DockIT

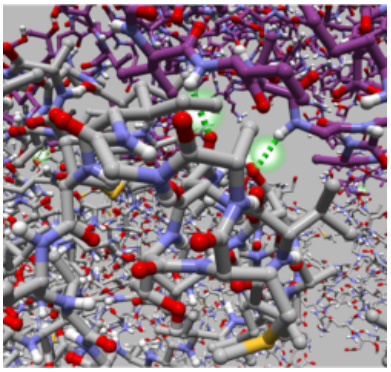
DockIT is a tool for interactive molecular docking

DockIT is software for interactive molecular docking. It enables the user to control the position and orientation of a ligand and a receptor bringing them into a docking pose either with a mouse and keyboard, with a haptic device or a VR headset (Oculus Rift, Rift S or Meta Quest2). Using a VR headset is the most immersive approach. Atomic interactions are modelled using molecular dynamics-based force-fields. It can be used for rigid docking and it also can be used incorporating receptor flexibility.

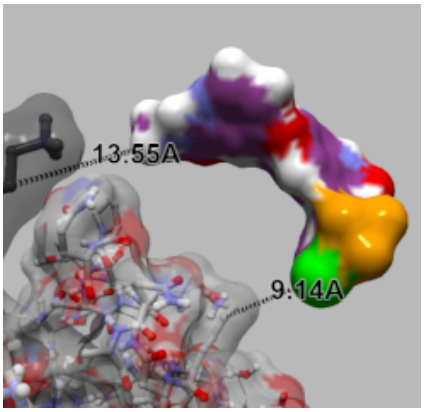
The following images are screenshots from the software.



GroEL and GroES. GroEL is rendered with ball-and-stick and semi-transparent molecular surface. GroES is rendered with the solid molecular surface.



The interatomic hydrogen bonds are depicted with green dashed lines.



Sorafenib and Braf. Dashed lines between atoms on each of the structures are shown to illustrate the distance between them.

An OpenCL enabled GPU is required to run the software.

If you have any feedback or issues using DockIT please email: info@dockit.uk

For further information please visit the DockIT site by clicking here

If you have any difficulties downloading the DockIT tool, please contact us.

References

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