A Free and Source-Available Rendering Workflow for Ligand Binding Conformity for Biochemical Engineering

ABSTRACT

Biochemical 3D rendering solutions have consistently remained behind the industry standard solutions present for 3D design often due to the specificity of their intended workload. Improving render quality would allow for more clarity and intentionality in figures present in publications and potentially improve scientific engagement during outreach programs and conferences. Unfortunately many of these 3D rendering solutions are both costly and time-consuming to learn, placing them firmly outside the reach of non-commercially focused entities such as academic laboratories or prospective students. This is especially hindering in areas of biochemistry which benefit heavily from visualisation, such as biochemical engineering and medicinal chemistry. In an effort to resolve this issue this report describes a methodology through which molecule binding conformities can be rendered at a quality exceeding the current industry standard and which is entirely cost-free, using source-available and open source solutions wherever possible.

METHODS

Docking & Conformity – AutoDock Vina and SwissDock

Desired ligand and target are virtually docked together using either SwissDock (*Bugnon et al 2024, Röhrig et al 2023*) or AutoDock Vina *(Eberhardt et al 2021, Trott & Olson 2010)*. AutoDock Vina is recommended due to the open-source aims of this report. SwissDock, whilst not open source, allows use of AutoDock Vina within its interface, or alternatively the proprietary attracting cavities docking mode. After determining likely binding conformities through examination of ΔG, AC and SwissParam scores, download or export the docking result. This will provide a ".dock4" or similar file.

As a worked example in this report porcine cathepsin H was docked with CA-074Me. The porcine cathepsin H structure was obtained from RCSB PDB (8PCH) *(Berman et al., 2000) (Guncar et al, 1997)* whilst the structure of CA-074Me was obtained from PubChem *(Kim S et al, 2025)(National Centre for Biotechnology Information, 2025).*

Initial Visualisation & Modification – PyMOL

By default, PyMOL *(Schrödinger & DeLano, 2020)* will not be able to import predictive docking files. Due to this, we must install the "PyViewDock" extension *(Boneta, 2021)*. After installing, import the docking file generated in the previous step by following the PyViewDock documentation. After import, you will see multiple frames imported by default, with each frame being a different binding conformity generated by your docking software. Select the desired binding conformity by selecting it's frame.

Here, any chemical modifications can be applied if necessary to your ligand. This should be limited to changes that do not alter the properties of the binding, such as removal of suspension or free hydrogens. If you wish to alter the chemical properties of the ligand, do so prior to docking using your favoured software to maintain predictive accuracy.

After making any necessary modifications, export the structure from PyMOL using the “”Export Structure,” and “Export Molecule” options, selecting all structures and using the frame selector to identify the conformity you wish to render. Export in the “PDBx/mmcif” format.

Final Modifications & Rendering – Blender

By default, Blender cannot import 3D data from the PyMOL outputted file format, so you must first install the Molecular Nodes extension *(Johnston, 2022)* in order to import your ligand into Blender. Consulting the Molecular Nodes documentation is strongly suggested hereafter. Import the PyMOL file using Molecular Nodes from local using the ball and stick method. Switch to rendered view. Here, you may notice geometry issues regarding the bonds. If this is the case, switch to the geometry nodes tab and locate the checkbox under named attributes “Find”. Enable this, and bonds should appear in the correct position.

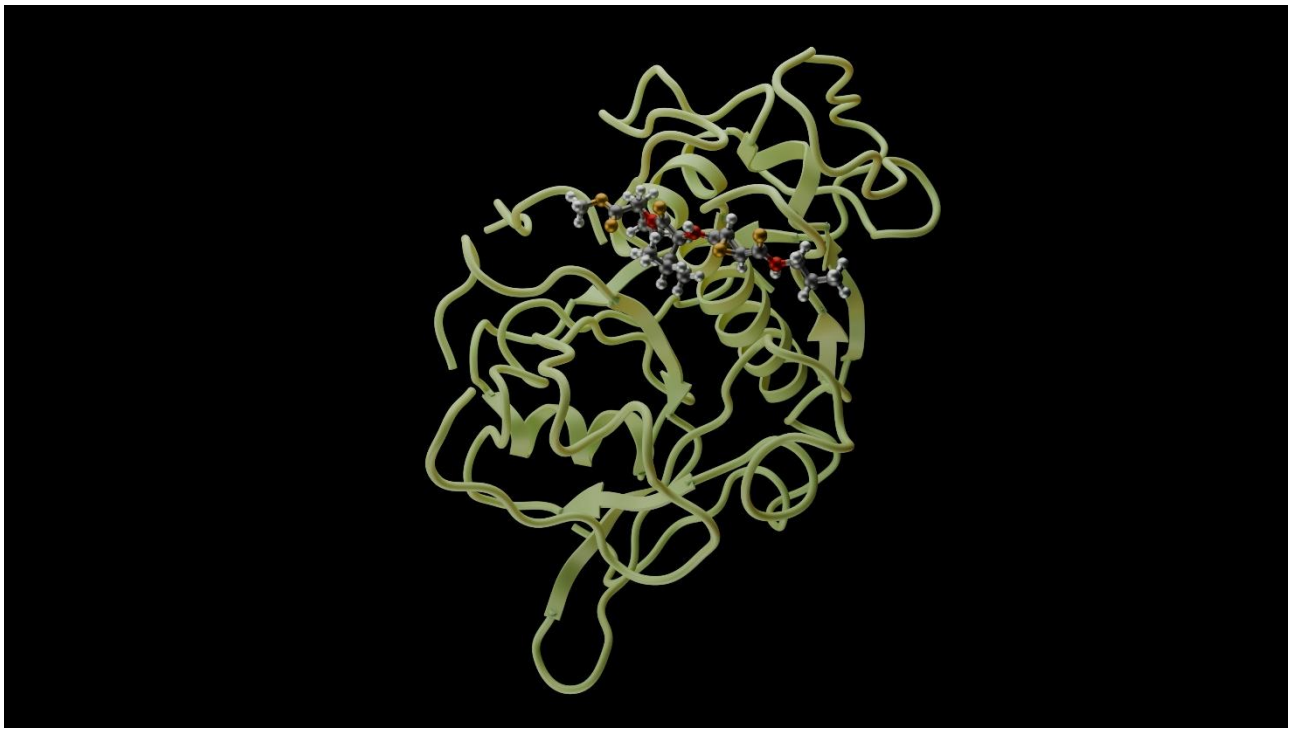
Next we must import the target. Once again, using Molecular Nodes import the .pdb of your target molecule from local – this time selecting the surface method. Alternatively, you can select other methods, some of which are pictured below in the results. Use the .pdb included in your docking output, as it will automatically scale and orient itself to the exact correct conformity as seen in PyMOL.

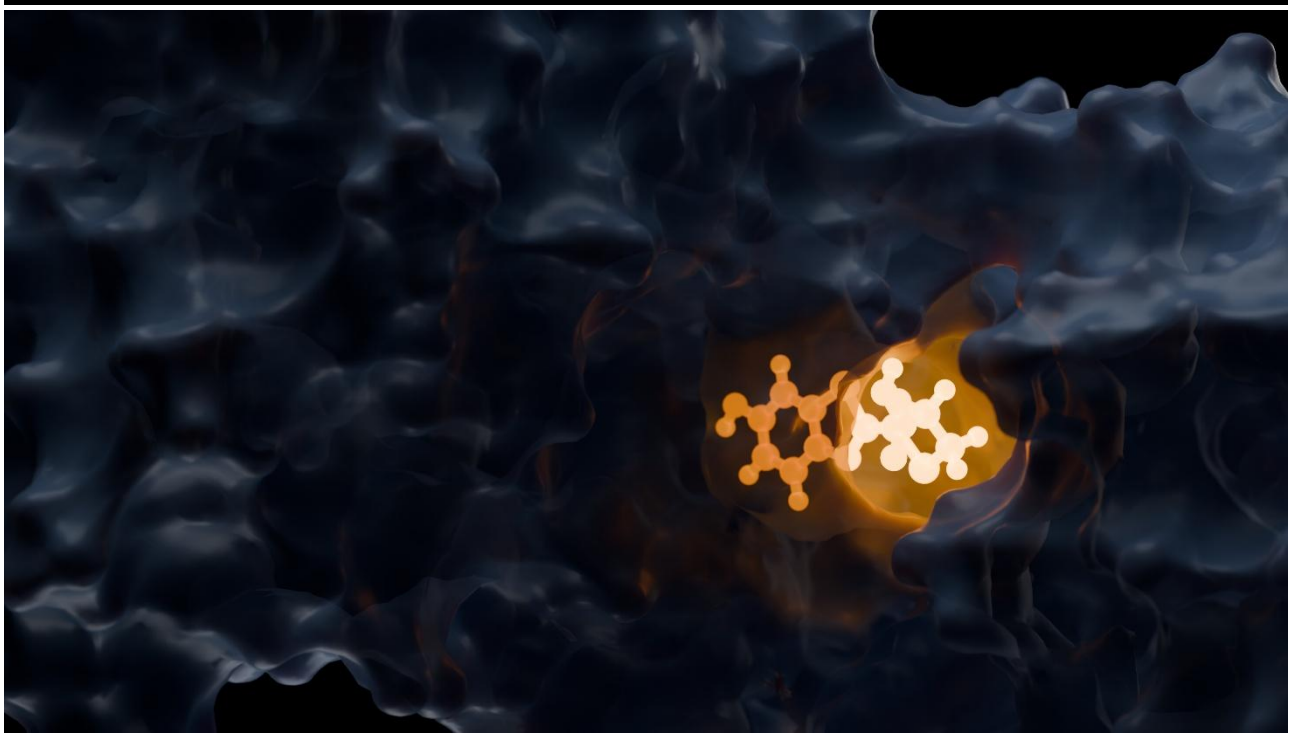
Here is where any subjective changes are made to both the target and ligand to prepare it for final render. This involves determining material, polycount, scene lighting, and camera position amongst a large quantity of other variables. If interested in tweaking the scene further consult the Blender documentation *(Blender Team, 2025)*.

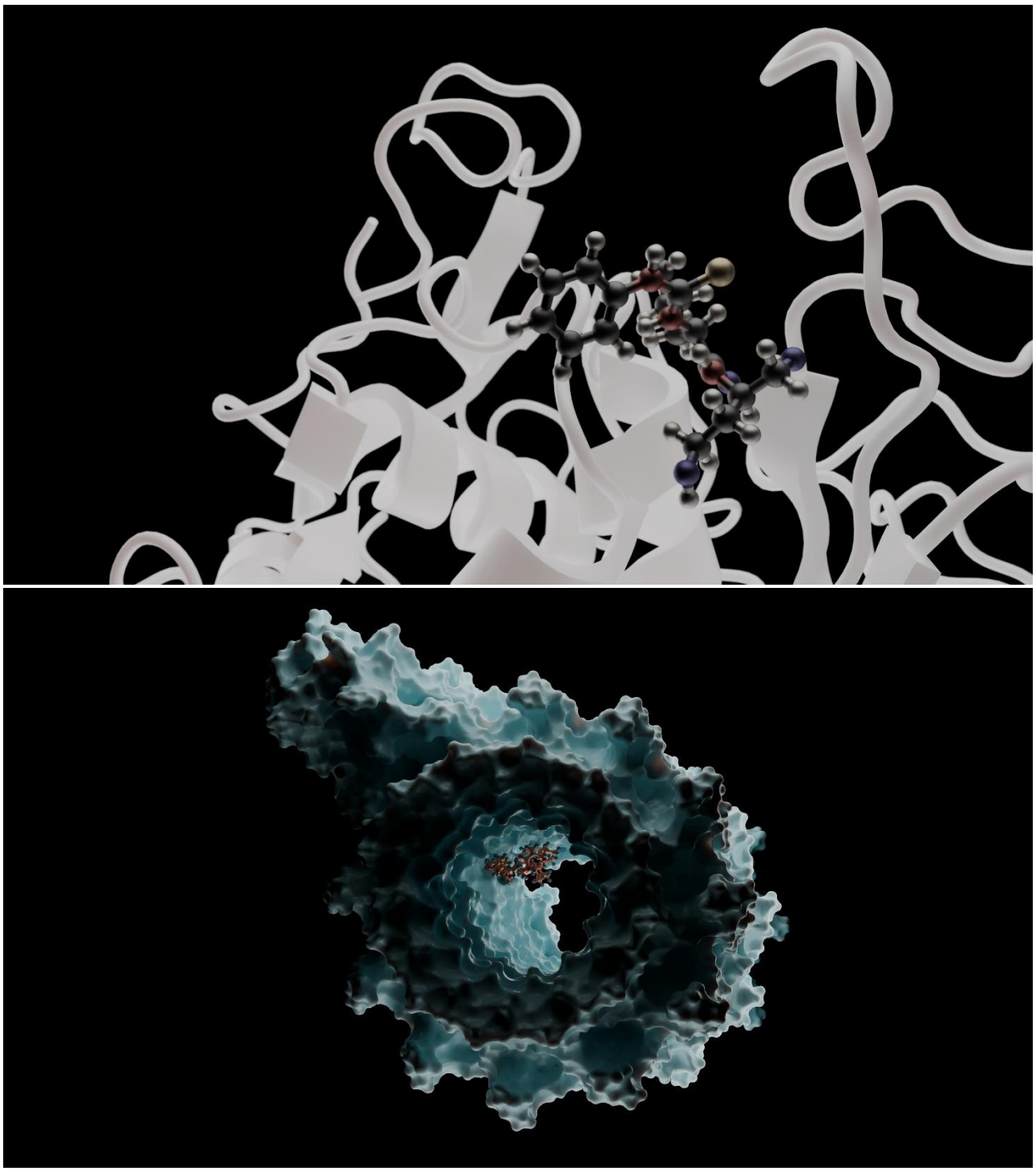
Rendering Multiple Conformities

You may wish to add another molecule binding to your ligand depending on conformity cluster predictions. In order to do this export the desired conformity from PyMOL as a .PDB and load it into Blender via molecular nodes alongside your first molecule and ligand. In order to determine the difference between the two molecules it is recommended you colour code them by assigning them different materials through the included geometry nodes presets. After this, render as described previously.

RESULTS







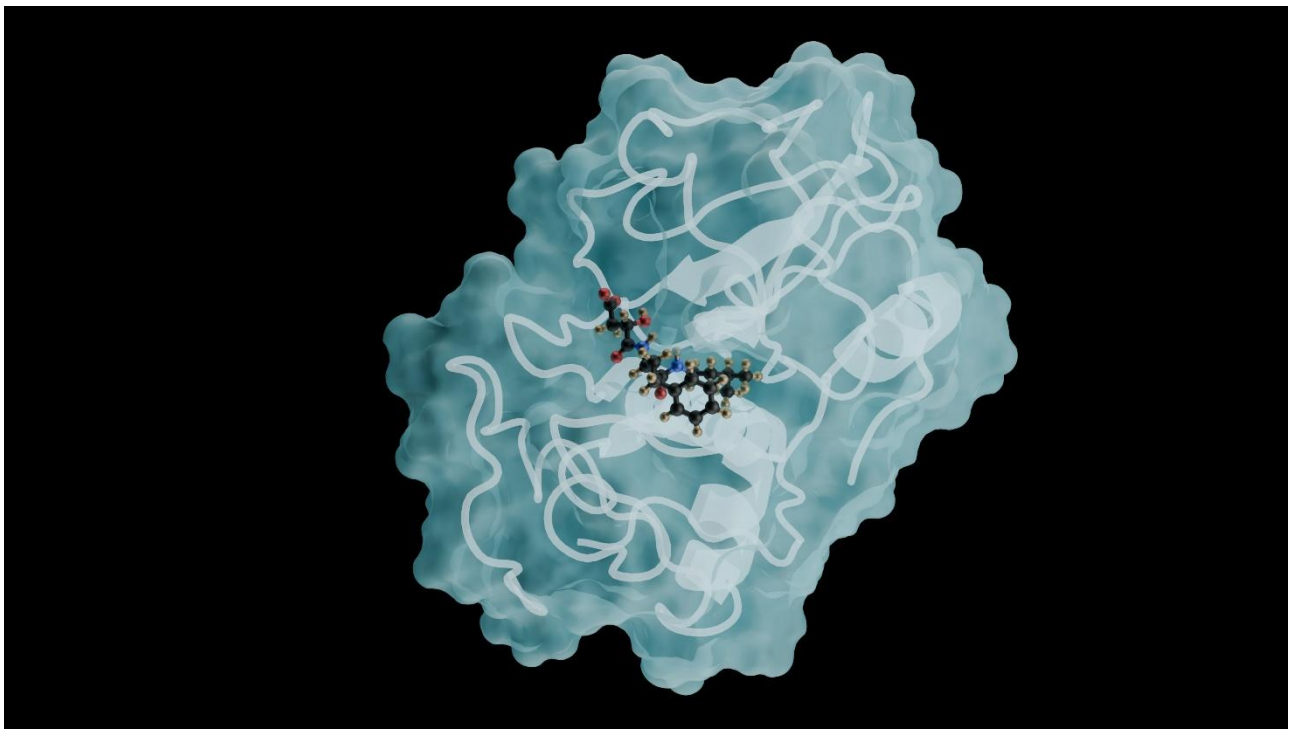


Figure 1 – A folio of renders made in Blender using Molecular Nodes and rendered in Cycles. In order of appearance: Cathepsin H predicted binding with CA074-Me, Firefly Luciferase predicted binding with D-Luciferin, Oligomycin predicted binding with ATP Synthase F_0 Subunit, SNJ-1715 predicted binding with Calpain-1 Catalytic Subunit, and WRR-99 predicted binding with Cruzipain.

As seen in *Fig. 1*, the resulting renders are of a significantly improved quality when compared to other rendering software alternatives such as Jmol and PyMOL. They also allow for much greater flexibility in presentation due to both scene and material control provided by Blender and Molecular Nodes – for example WRR-99 can have both it's surface and cartoon represented simultaneously. Transparency and emission can also be used to better show internal binding sites, as seen with the Firefly Luciferase predicted binding with D-Luciferin.

These renders are available in full size (3840x2160) in the GitHub repository alongside brief animations meant to emulate introductory conference slides.

DISCUSSION

I believe that the renders shown in *Fig. 1* illustrate a clear quality improvement in favour of the Blender render workflow compared to traditional methods. Given that this entire pipeline is either source-available or open-source and entirely free to implement, it seems it could be used in a myriad of ways for biochemical renders. This includes both students and professionals given the prevalence and ease-of-use of Blender and PyMOL.

Another aspect where blender also shows drastic improvements over PyMOL or Jmol is granularity and control. Not only can you modify the appearance of the molecule and protein, but the scene around them to better incorporate them into presentations or publications as necessary. This pipeline could also be modified to fit medicinal chemistry modification to better communicate novel structures.

Regarding drawbacks, the only significant one is rendering time. For rendering still images, the time difference is negligible compared to other solutions if using GPU-accelerated rendering. Without this capability, however, rendering times would increase significantly. As an alternative, Blender includes a less strenuous renderer – EEVEE *(Blender Team, 2025)*, which can easily be run on limited hardware and provides a less detailed render. Despite this slight limitation, you still gain all of the granular control inherent to working in Blender when compared to other software, and renders maintain a very high quality.

To conclude, I believe that this report has clearly shown the merits of this rendering pipeline and the vast majority of this must be attributed to the extremely talented developers of Molecular Nodes, PyViewDock, AutoDock Vina, PyMOL and Blender. Open-source and source-available software is vital in the educational ecosystem and the accessibility of each of these programs makes it possible to drastically improve render quality and improve communication.

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