

Ensuring accurate modeling in its electron density of a ligand bound to a therapeutic target in a high throughput environment: a review of best practices

Thierry Fischmann

Merck

Accurate modeling of a ligand in the electron density map is critical to a structure-based drug design project. Indeed it impacts the understanding of the interactions of the ligand with its binding site. It also impacts further modeling of new substituents. However the need for correctness competes with the requirement to deliver structures in a timely fashion. In this presentation we will review some of the tools and best practice workflow that are commonly used in a high throughput environment to ensure the accuracy of a structure while at the same time minimizing the need for time-consuming checks