Nuclear magnetic resonance (NMR) techniques combined with computational methods such as docking and cheminformatics were used to characterize protein structure and ligand binding. The thioredoxin system of *Mycobacterium tuberculosis* consists of a thioredoxin reductase and at least three thioredoxins. This system is responsible for maintaining the cellular protein thiol redox state in normal state. This maintenance is important as the bacterium is engulfed by the human macrophage. Here it is bombarded by reactive oxygen and nitrogen species in an attempt to disrupt normal cellular function in part by perturbing the protein thiols. To this end, the solution structures of the three thioredoxins, A, B, and C, in the oxidized state were solved by NMR. Additionally, the reduced form of thioredoxin C was solved as well. Docking and NMR chemical shift perturbation experiments show promise for the inhibition of the thioredoxin C-thioredoxin reductase catalytic turnover.

Automated docking is the process of computationally predicting how tightly a ligand binds to a protein and the correct orientation. The docking of an in-house collection of 10,590 chemicals into a protein called dual specificity phosphatase 5 identified potential ligands. These compounds were characterized as inhibitors in a phosphatase assay and as ligands in NMR chemical shift perturbation experiments. Based on a promising lead compound, additional chemicals were identified using cheminformatics and subjected to the same experimental verification.