The human dopamine D1 receptor is involved in movement, reward and reinforcement, learning, and memory. As such, it is an important target for Parkinson’s disease and treatment of drug addiction. A plausible structure for D1 was predicted using portions of the new Membstruk procedure. However, prediction of ligand docking with the standard MSCDock procedure met with limited success.

Due to the poor results from the old MSCDock procedure, the D1 system was used as a test case for improving the MSCDock procedure, resulting in a procedure called GenMSCDock. When applied to the D1 system, portions of this procedure showed improved results and suggest that full use of GenMSCDock will result in further improvements. For example, the ligand conformation shown below would not have shown up in the final set of results when using the old procedure. Because the full GenMSCDock procedure has not been applied to D1, the current docking results are considered preliminary. A full study of D1 using GenMSCDock is forthcoming.

When full docking studies of D1 using GenMSCDock have been finished, the structure of the dopamine D5 receptor, which is closely related to D1, will be predicted using the finalized version of the new Membstruk procedure, and docking studies will be performed using the new GenMSCDock procedure.