Several modifications to the standard MSCDock procedure were tested on the human dopamine D1 system and have since been incorporated into a new docking program, GenMSCDock, which uses MSCDock as its core. One of the main improvements to MSCDock is the implementation by John Wendel of a Voronoi clustering algorithm to re-cluster the initial MSCDock structures. Another improvement is the ability to easily alanize and dealanize the protein before and after docking. Alanizing refers to the replacement of bulky nonpolar residues with alanines, thus allowing the ligand to sample a larger space during docking. Following docking the protein is dealanized, which means that the bulky residues are replaced. The last major improvement is the ability to neutralize the protein-ligand complexes with relative ease. This is a step that, due to its difficulty, was left to the end in the old procedure. It can now be performed immediately after the dealanization step, thus removing or reducing long range coulomb interactions, one of our largest sources of error and bias.

The modular nature of GenMSCDock should make it easy to maintain and add new functionality. Additionally, the flexibility of the program will allow each user to easily tailor the procedure to their particular system while obtaining results that are consistent with the results of other systems. GenMSCDock will increase the accuracy of our docking studies while making it easier to perform those docking studies.