

MolMover.xls is a two page spreadsheet. The first page, when saved as space delimited text (*.prn), produces a file in PDF format. The second page is used to rotate and translate the coordinates. Z-axis rotation is entered in cell J2, X-axis rotation cell N2, Y-axis rotation in cell R2. These rotations are performed in this order. X, Y, Z translations are entered in cells U3, V3, and W3.

There is also a feature whereby the best rotations and translation to fit your molecule to a target can be found. You have to add target atoms in register with their corresponding atoms in the structure. The use the "Solver..." under the TOOLS menu to perform a nonlinear least-squares fit of the rotations and translations to fit the two molecules. The sum of the squared residuals in cell AK3 is minimized. The resultant coordinates are pasted into the first page using "paste values" and saved as a *.prn file. Warning: Do not change the column spacing as that will put the pdb file out of register.

The example in the sheet moves a 20 base-pair segment of DNA to overlap with target sugars at the base pair of residues 1 and 20.