Table S1: Cluster analysis of MD simulations of enzyme-structure complexes

Cluster	_(2R,3R)_			_(2S,3S)_			_(2S,3R)_		
	Frames	$RMSD_{initial}$(Å)	$RMSD_{Mini}$(Å)	Frames	$RMSD_{initial}$(Å)	$RMSD_{Mini}$(Å)	Frames	$RMSD_{initial}$(Å)	$RMSD_{Mini}$(Å)
0	429(65%)	0.948	0.0588	460(71%)	0.967	0.0619	226(34%)	1.245	0.0636
1	195(30%)	1.057	0.0558	103(16%)	1.097	0.0613	201(30%)	1.21	0.0608
2	13(2%)	1.23	0.0609	85(13%)	1.202	0.0581	165(25%)	1.216	0.0627
3	12(2%)	1.29	0.0596	10(2%)	1.294	0.0567	53(8%)	1.298	0.0607
4	11(2%)	1.239	0.0595	2(1%)	1.301	0.0586	15(2%)	1.532	0.0625

RMSD analysis was performed on all atoms for each structure;

$RMSD_{initial}$: The deviation of cluster coordinates to the initial structure coordinates;

$RMSD_{Mini}$: The deviation of minimized structure coordinates (used for QM/MM scan) to their respective cluster coordinates