



Figure S1. Evolution of $C\alpha$ -rmsd (\AA) with time for all of the WT (yellow, B), A52T (blue, C), A22S (green, D), and V108M (red, E) COMT simulations performed at 25°C (A) and 37°C (B-E). Simulations of COMT beginning with crystal structures of the human WT (PDB entry 3BWM (54)) and V108M (PDB entry 3BWY (54)) proteins are colored in black and included for comparison with simulations using the homology models.