

CFTR/BSc3596

CFTR/diketo curcumin

closed  
channel

open  
channel

CFTR/keto-enol curcumin

CFTR/diketo curcumin

8 Å

CFTR/BSc3596

CFTR/keto-enol curcumin

**Figure S1. RMSD traces of the MD simulations.** RMSDs calculated on the CFTR conformer backbone atoms aligned to the parent PDB structures kickstarting the MD simulations (closed CFTR, PDB 5UAK; open CFTR, PDB 6MSM). The closed channels exhibit greater RMSD fluctuation than the open channels owing to the higher conformational freedom of the former (undimerized NBDs) with respect to the latter (dimerized NBDs).