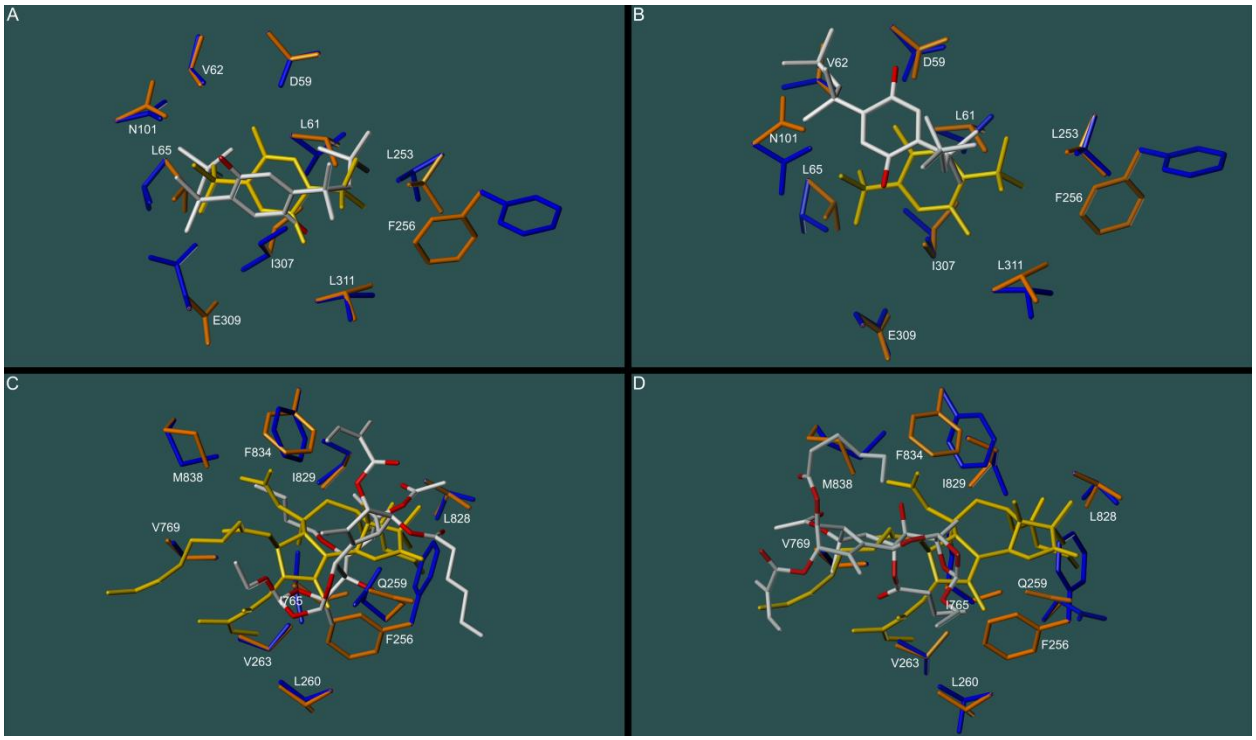
Supplementary Materials



Docking-predicted conformational changes in the binding sited upon binding of a bulky BHQ analog (2,5-bis-(1',1',3',3'-tetramethylbutyl)-benzene-1,4-diol; panels A and B) and a large TG analog with an additional five-membered ring (compound **7** in the original report (Nielsen, Thastrup et al. 1995); panels C and D). Docking was performed with GOLD/GoldScore (panels A and C) and AutoDock (panels B and D), showing the extent of deviations of computed side chain (blue) and ligand positions (CPK colored) from the X-ray crystal structure (orange and yellow).