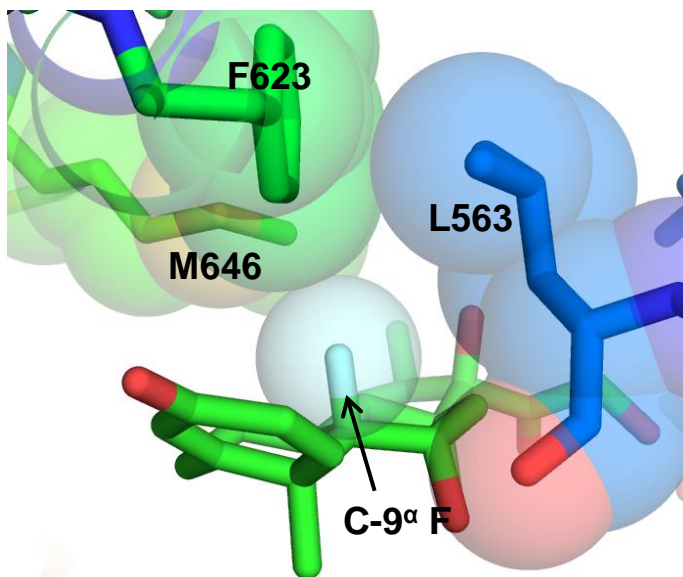
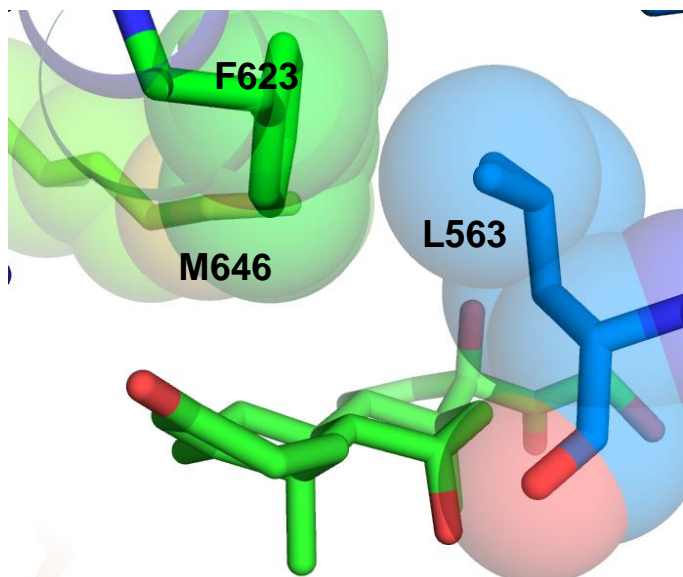
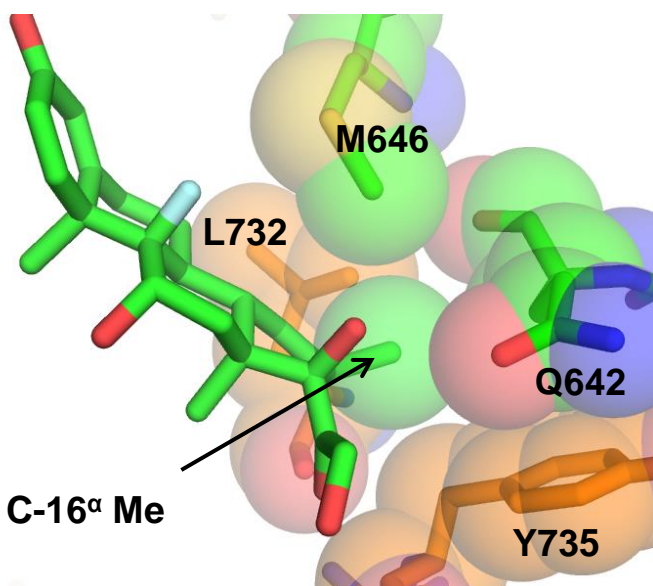
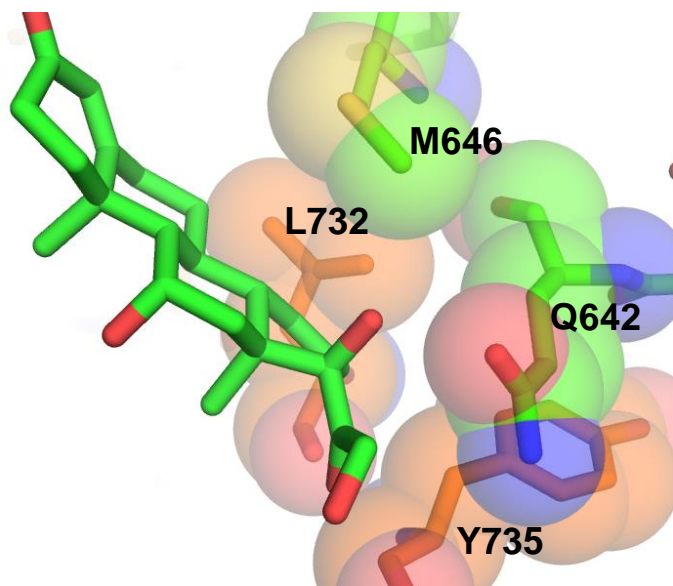


A**DEX-bound GR LBD****Cortisol-bound GR LBD****B****DEX-bound GR LBD****Cortisol-bound GR LBD**

Supplementary information, Figure 5. Detailed structural comparisons of the steroid C-9 α group and C-16 group of Dex and cortisol in the ligand binding pocket of the GR LBD. (A) The F atom at the C-9 α position of DEX makes a close contact with F623, L563 and M646 in the ligand binding pocket of GR LBD. (B) The C-16 methyl group of DEX makes close contacts with Y735, L732, M646 and Q642 in the ligand binding pocket of the GR LBD.