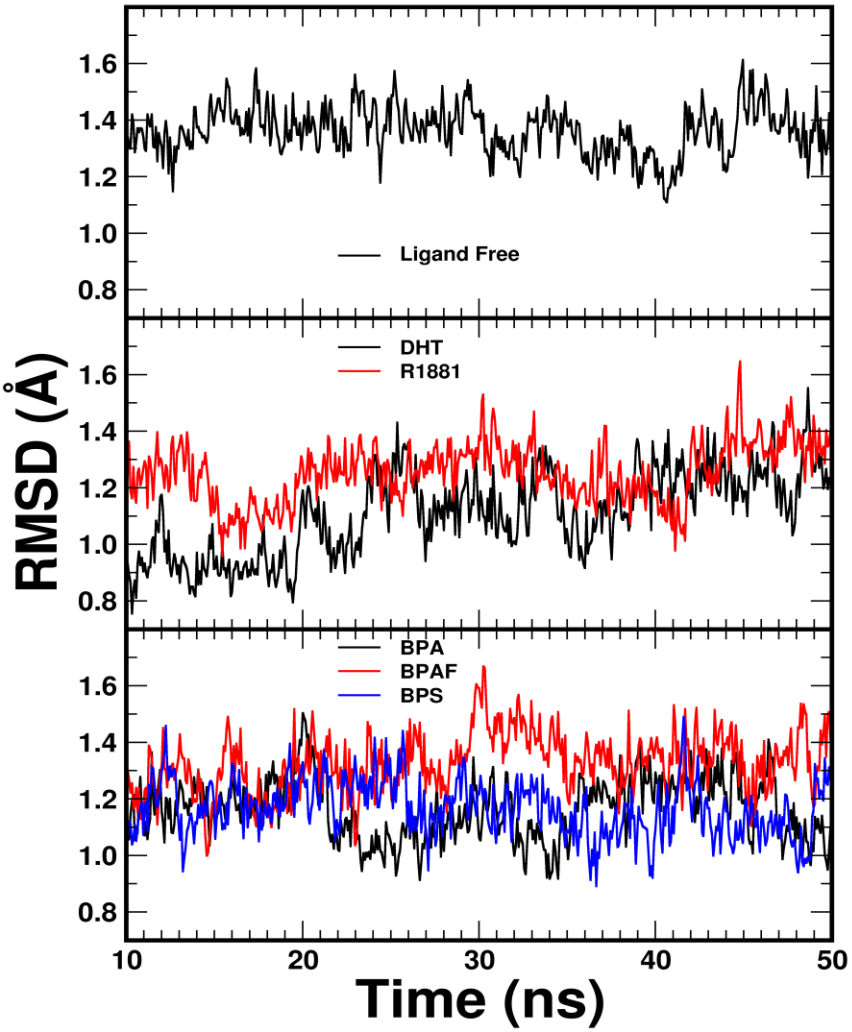
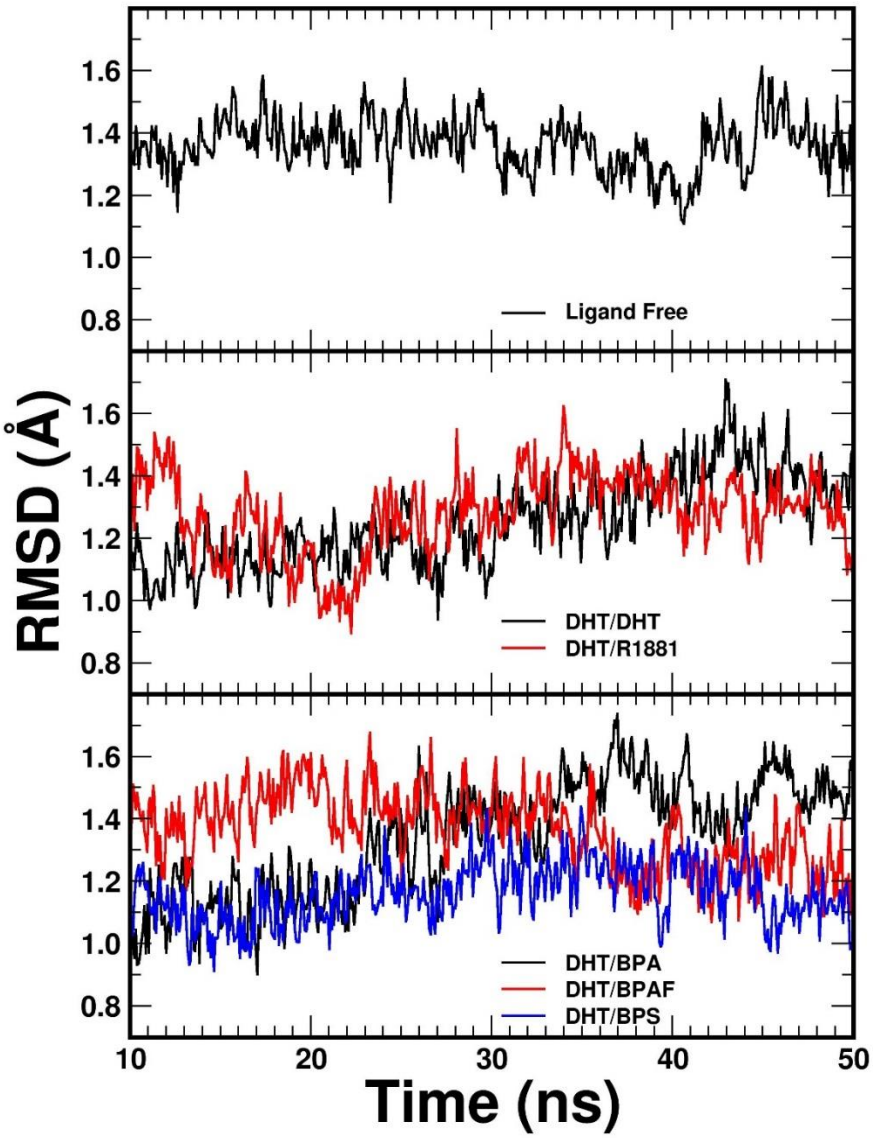
Supplementary material

Binding of bisphenol A, bisphenol AF, and bisphenol S on androgen receptor: Coregulator recruitment and stimulation of potential interaction sites

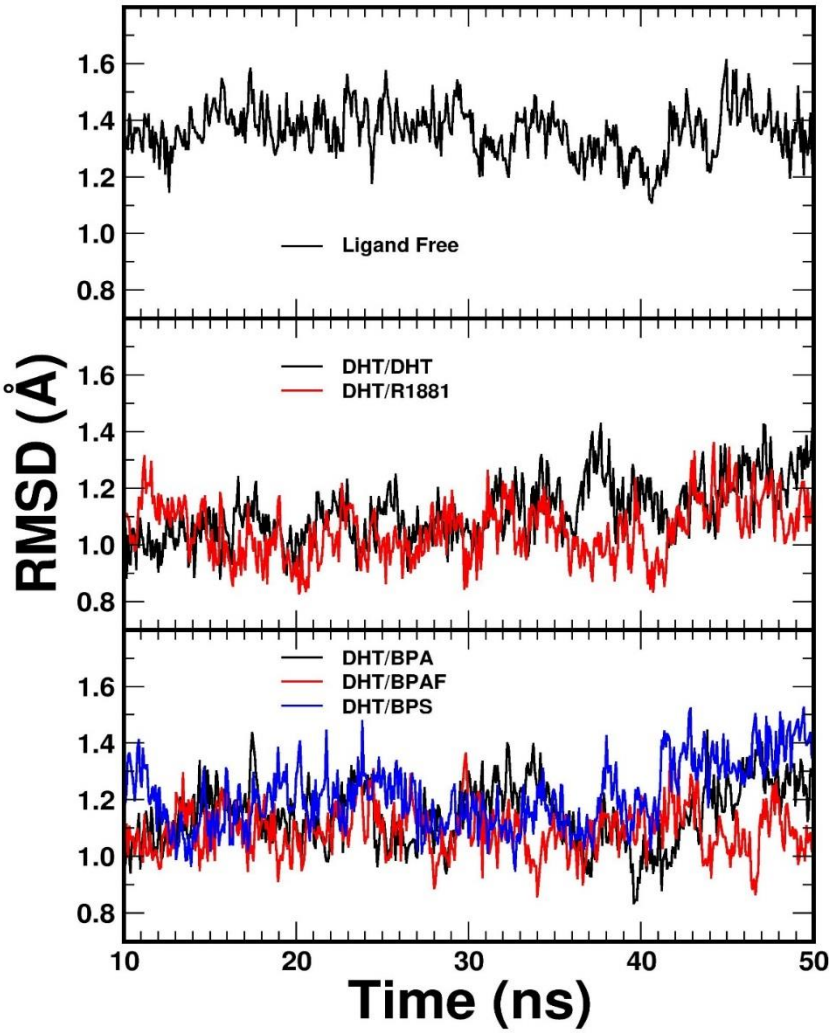
Lalith Perera, Yin Li, Laurel Coons, Rene Houtman, Rinie van Beuningen, Bonnie Goodwin, Scott Auerbach, and Christina Teng



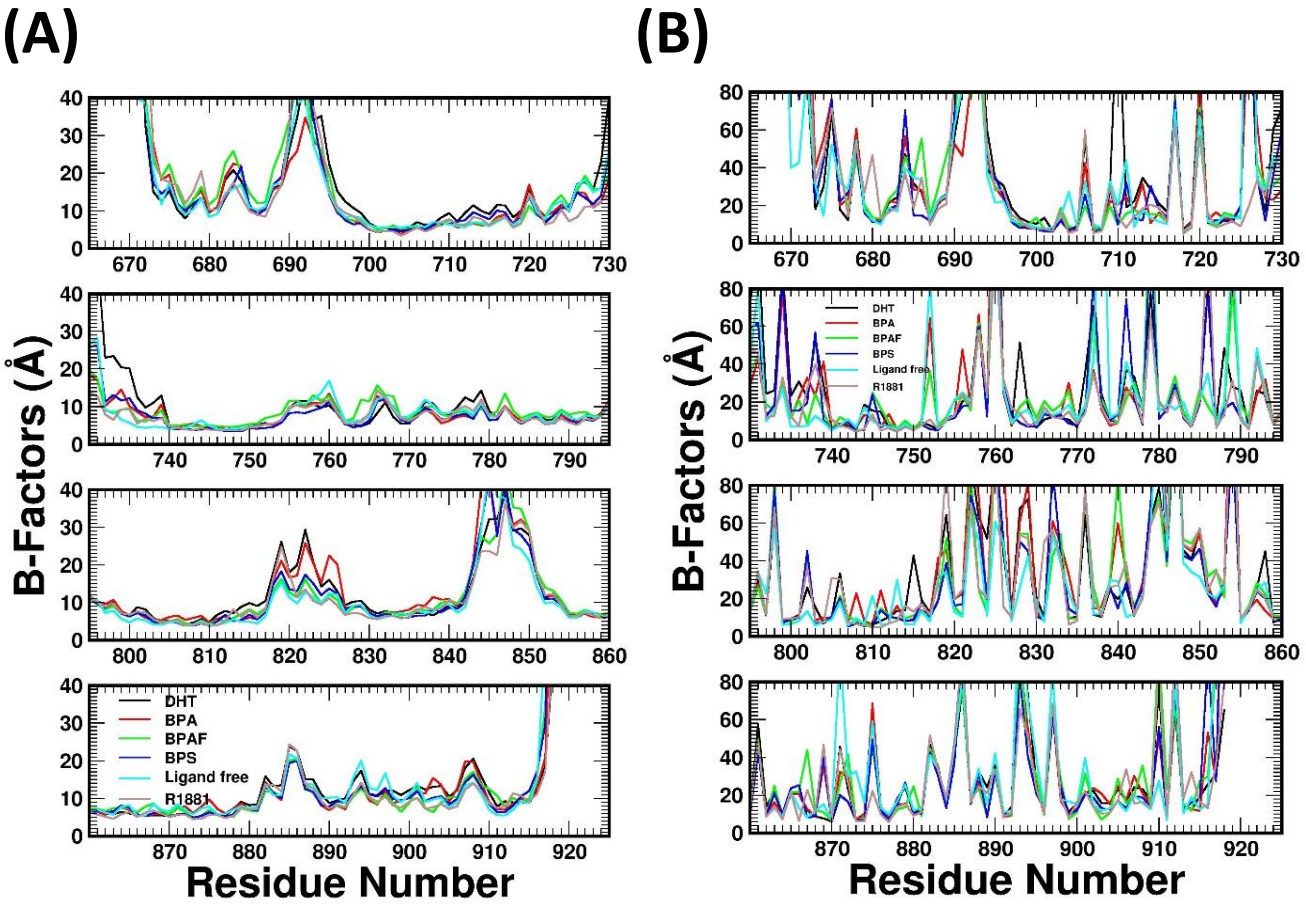
Supplemental Fig. 1. Root mean square deviation of various ligand bound AR structures in which ligand is at the regular ligand binding site. The X-ray crystal structure (pdb ID: 3L3X) was used as the reference structure for these calculations and all backbone heavy atoms of each residue were used to calculate the averaged RMSD at each time point.



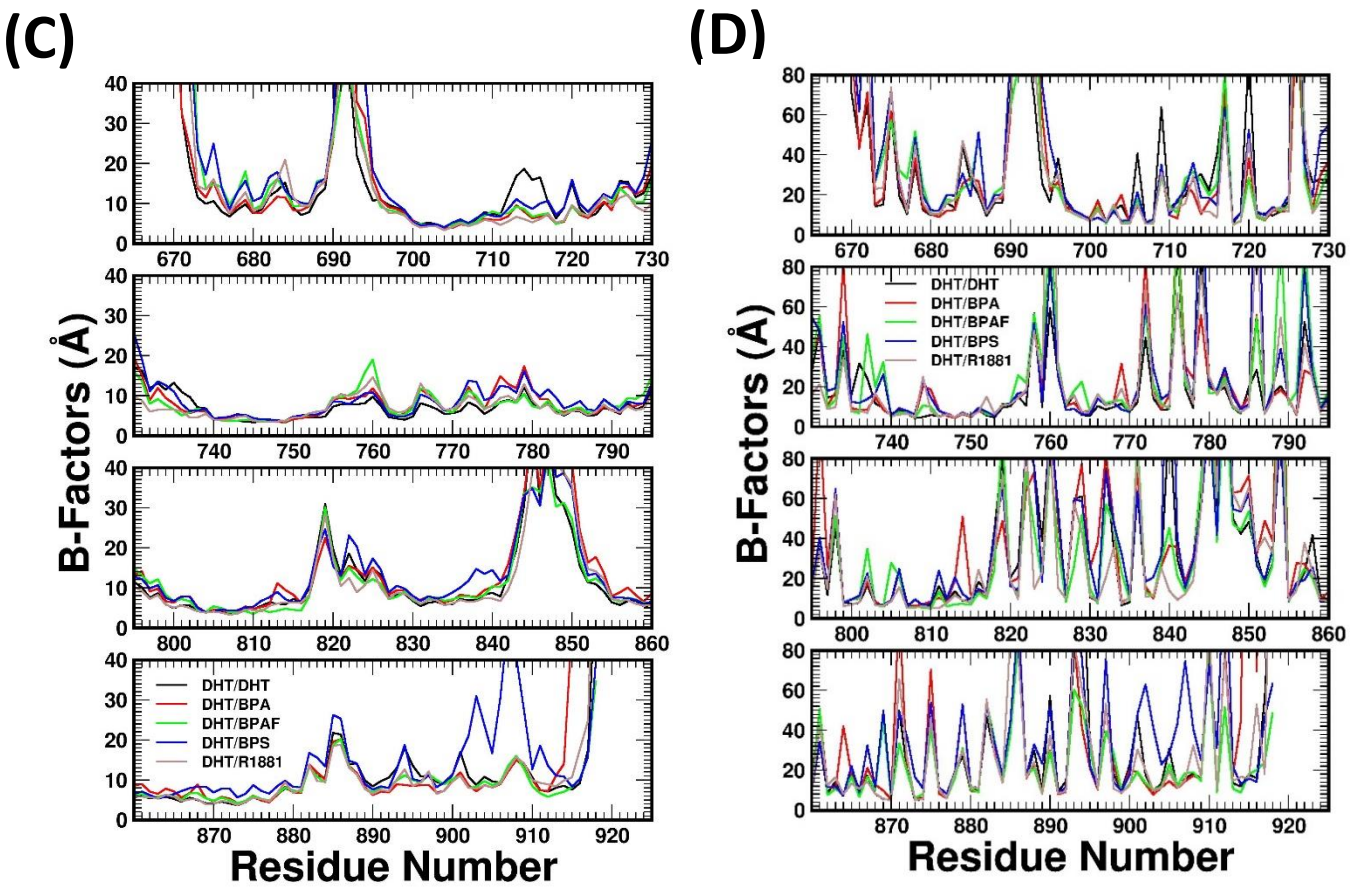
Supplemental Fig. 2. Same as S Fig. 1, but for the structures with the AF2-site bound ligand. In addition, DHT is bound at the natural ligand binding site in all systems.



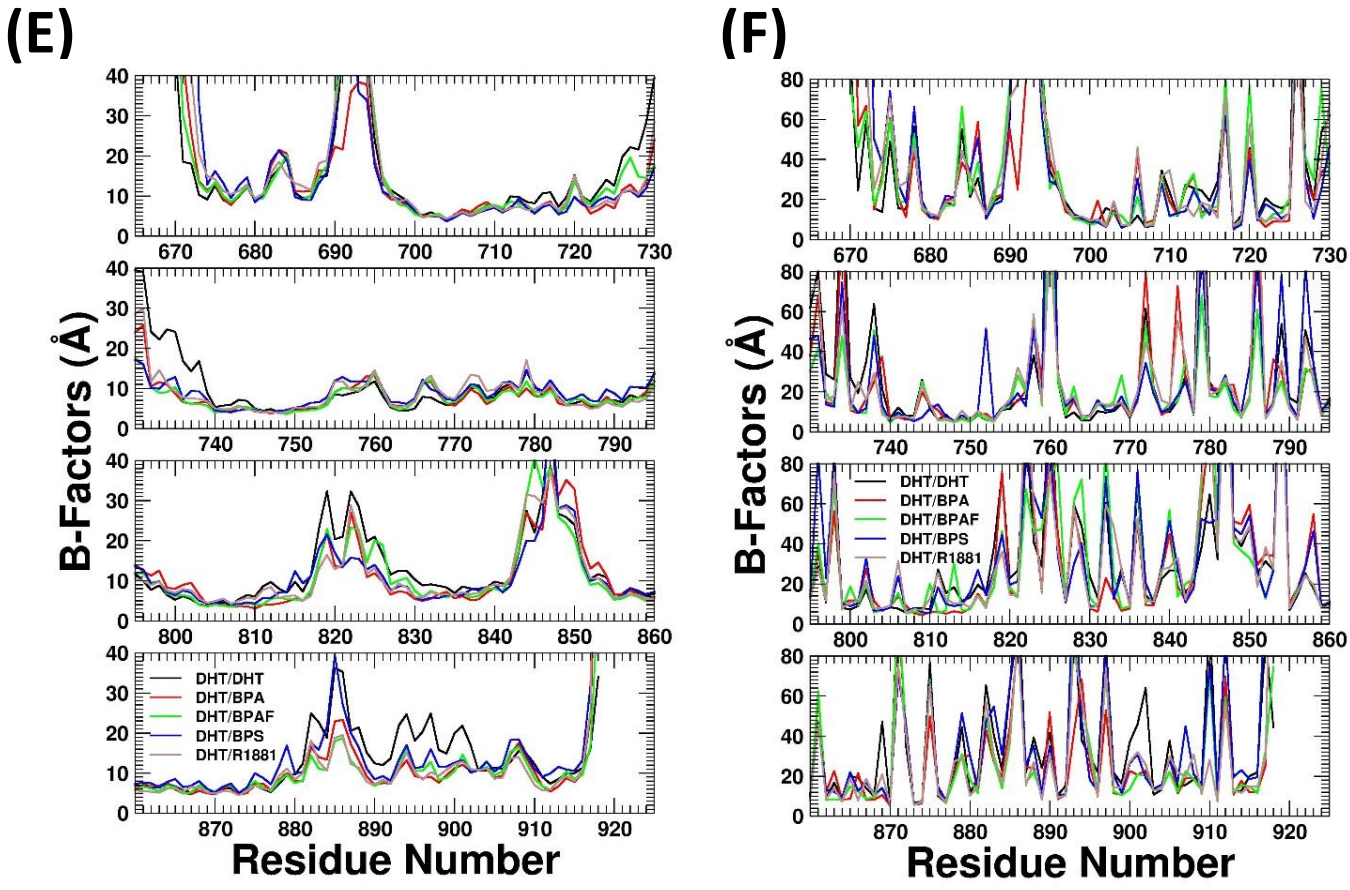
Supplemental Fig. 3. Same as S Fig. 1, but for the structures with the BF3-site bound ligand. In addition, DHT is bound at the natural ligand binding site in all systems.



Supplemental Fig. 4. B-factors representing the average fluctuations of atomic positions calculated from backbone atoms (panels A, C, and E) and the side chain heavy atoms (panels B, D, and F) averaged over the last 40 ns of each trajectory for each system. In A and B, ligands that bind to the regular ligand-binding site (LBS). B-factors for the ligand free AR are also shown (in cyan). In C and D, ligands are at the AF2-site in addition to DHT at the natural LBS. In E and F, ligands are at the BF3-site in addition to DHT at the natural LBS.



Supplemental Fig. 4. – continued



Supplemental Fig. 4. – continued