Bisphenol A analogues (BPAs) belong to a wide variety of large volume chemicals with diverse applications yet emerging environmental concerns. Limited experimental data have demonstrated that BPAs with different halogenation patterns distinctly affect the agonistic activities toward proliferator-activated receptor (PPAR)γ and estrogen receptors (ER)α. Understanding the modes of action of BPAs toward different receptors is essential, however, the underlying molecular mechanism is still poorly understood. Here we probed the molecular recognition process of halogenated BPAs including TBBPA, TCBPA, BPAF, BPC, triBBPA, diBBPA, and monoBBPA toward PPARγ and ERα by molecular modeling, especially the impact of different halogen patterns. Increasing bromination at phenolic rings of BPAs was found highly correlated with electrostatic interactions (R^2 = 0.978 and 0.865 toward PPARγ and ERα, respectively) and van der Waals interactions (R^2 = 0.995 and 0.994 toward PPARγ and ERα, respectively). More halogenated phenolic rings at 3,5-positions of BPAs increase the shielding of the hormonally active phenolic OH and markedly decrease electrostatic interactions favorable for agonistic activities toward PPARγ, but unfavorable for agonistic activities toward ERα. The halogenation at the phenolic rings of BPAs exerts more impact on molecular electrostatic potential distribution than halogenation at the bridging alkyl moiety. Different halogenations further alter hydrogen bond interactions of BPAs and induce conformational changes of PPARγ ligand binding domain (LBD) and ERα LBD, specifically affecting the stabilization of helix H12 attributable to the different agonistic activities. Our results indicate that structural variations in halogenation patterns result in different interactions of BPAs with PPARγ LBD and ERα LBD, potentially causing distinct agonistic/antagonistic toxic effects. The various halogenation patterns should be fully considered for the design of future environmentally benign chemicals with reduced toxicities and desired properties.