

Description of Additional Supplementary Files

Supplementary Movie 1 The overall structure of AHR-ARNT-DNA complex. AHR and ARNT PAS-B domains are spatially distant from other AHR and ARNT segments.

Supplementary Movie 2 The spatial distribution of eight AHR residues involved in direct interactions with six ligands. All six ligands are located at similar positions in the AHR PAS-B domain. H289, F293, G319, C331, F349, L351, S363, and Q381 are involved in interactions with all these ligands.

Supplementary Movie 3 The interaction network of R396 with D327 and V348. Ligand binding induces the outward movement of residues V348 and F349 on the G β strand. This movement facilitates the formation of a hydrogen bond between V348 and R396 on the J α helix. Additionally, R396 forms a salt bridge with D327 on the F α helix.

Supplementary Movie 4 The conformational change of C-ter loop during AHR's interaction with XAP2 or ARNT. Ligand binding to the AHR PAS-B domain induces a conformational change in the C-terminal loop, orienting it towards AHR and thereby reducing its interaction with XAP2. Subsequently, upon ARNT binding to AHR, the C-terminal loop facilitates heterodimeric interactions, leading to dissociation of XAP2 from the complex.

Supplementary Data 1 The MD simulation input, output and parameter files.