

Supplemental Information

Influence of the length and positioning of the antiestrogenic side chain of endoxifen and 4-hydroxytamoxifen on gene activation and growth of estrogen receptor positive cancer cells.

Philipp Y. Maximov, Daphne J. Fernandes, Russell E. McDaniel, Cynthia B. Myers, Ramona F. Curpan and V. Craig Jordan

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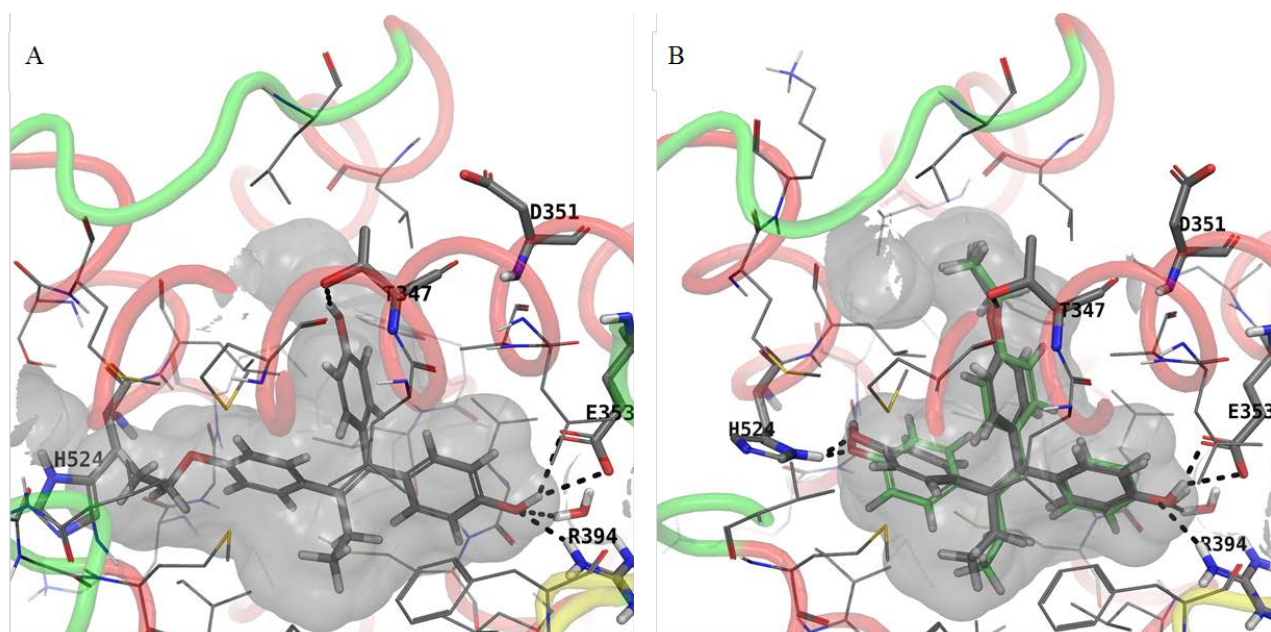


Figure S1. The representation of the agonist structure, 3Q97, binding site with the co-crystallized isomers, E-isomer of ethoxytriphenylethylene (A) and Z-isomer of ethoxytriphenylethylene (B). It can be seen the differences between the binding pocket when these isomers are accommodated.

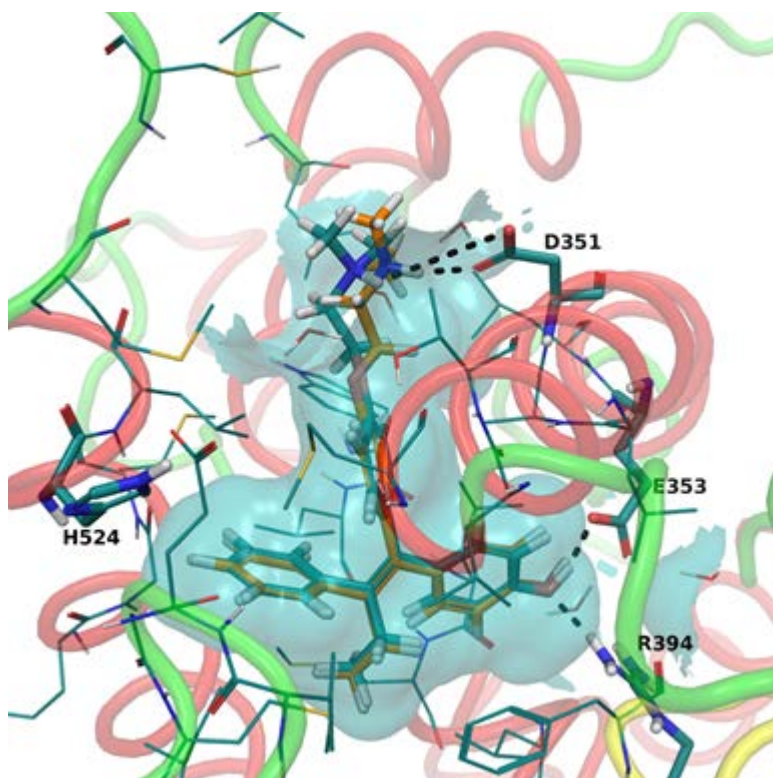


Figure S2. The top ranked docking pose of 4OHT superimposed with the native ligand in the experimental structure, 3ERT.

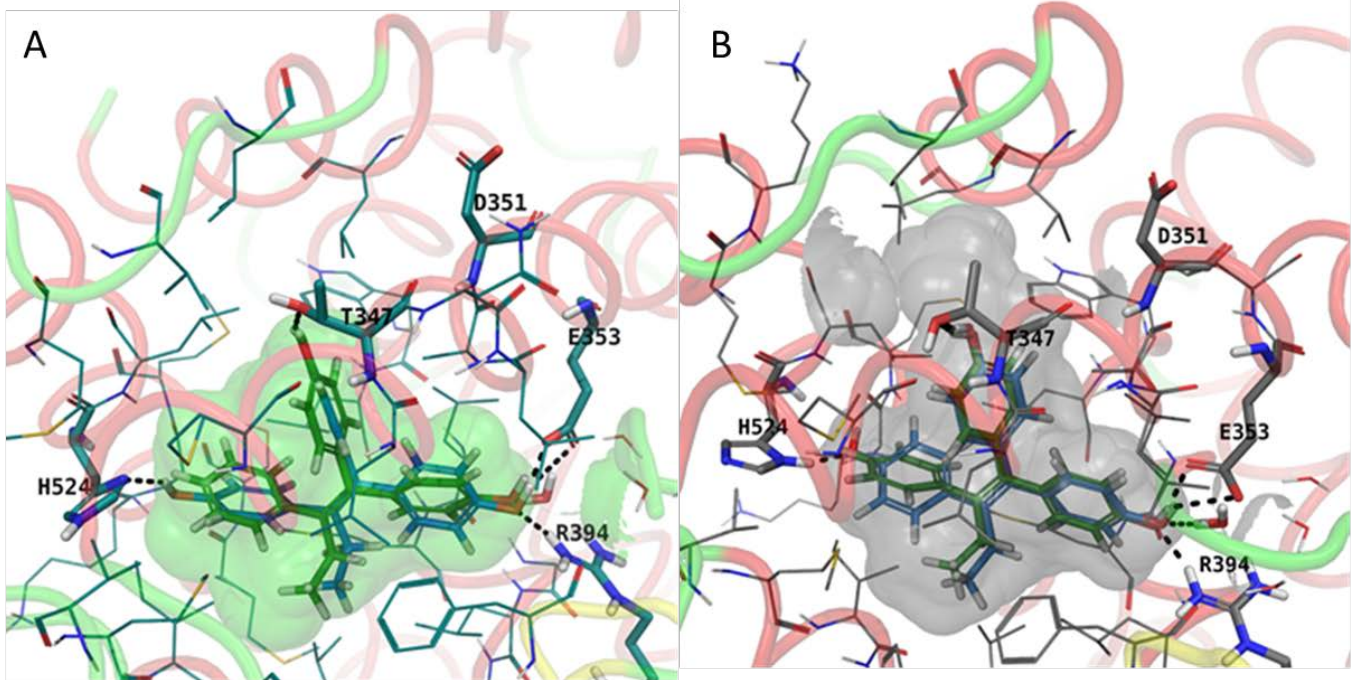


Figure S3. Docking poses of 3OHTPE (blue) and BPTPE (green) in the binding pocket of 1GWR (A) and 3Q97(B)