**Supporting Table S1. Autodock binding energy evaluation of 5AR homology model in complex with different substrates (kcal/mol)**

| SUBSTRATES | ENERGY |
|---|---|
| ***$NADP^+$*** | -9 |
| ***$NADP^+$ + testosterone*** | -8 |
| ***$NADP^+$ + finasteride*** | -9 |
| ***$NADP^+$ + beta-sitosterol*** | -11 |
| ***$NADP^+$ + stigmasterol*** | -9 |
| ***$NADP^+$ + campesterol*** | -10 |
| ***$NADP^+$ + daucosterol**** | -10 |
| ***$NADP^+$ + oleic acid*** | -8 |
| ***$NADP^+$ + lauric acid*** | -8 |
| ***$NADP^+$ + linoleic acid*** | -9 |
| ***$NADP^+$ + palmitic acid*** | -8 |

*Bound in different site