Biochem. J. (2014) **462**, 163–171 (Printed in Great Britain) doi:10.1042/BJ20140220

online data

SUPPLEMENTARY ONLINE DATA

Rate of steroid double-bond reduction catalysed by the human steroid 5β-reductase (AKR1D1) is sensitive to steroid structure: implications for steroid metabolism and bile acid synthesis

Yi JIN*, Mo CHEN* and Trevor M. PENNING*[1]

*Center of Excellence in Environmental Toxicology and Department of Pharmacology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA 19104, U.S.A.

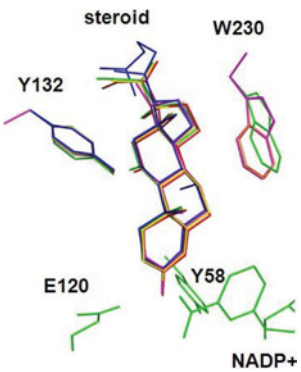

Figure 1 Comparison of the binding of steroids in AKR1D1

The docked conformations with lowest energy for testosterone (yellow), cortisone (green) and 7α-hydroxycholestenone (blue) are shown. The steroid A ring is buried in the active site with the Δ^4-double bond in close proximity to the catalytic tetrad (Glu^{120} and Tyr^{58} are shown) and the cofactor. The C17 side chain of the steroids protrudes out of the cavity. The details of the docking are given in the Experimental section of the main text. During docking, the side-chains of Tyr^{132} and Trp^{230} were kept flexible. The docked conformation of cortisone was identical with its conformation in the crystal structure of the AKR1D1–$NADP^+$–cortisone complex (PDB code 3CMF) (in magenta).

Received 14 February 2014/30 May 2014; accepted 4 June 2014
Published as BJ Immediate Publication 4 June 2014, doi:10.1042/BJ20140220

[1] To whom correspondence should be addressed (email penning@upenn.edu).