Albumin-directed stereoselective reduction of 1,3-diketones and β-hydroxyketones to \textit{anti} diols

Federico Berti,* Simone Bincoletto,a Ivan Donati,b Giampaolo Fontanive,a Massimo Fregonese,a and Fabio Benedetti*

\textit{a} Department of Chemical Sciences, University of Trieste, via Giorgieri 1. 34127 Trieste (Italy).
Fax: +39 040 5582402; E-mail: fberti@units.it; benedett@units.it

\textit{b} Department of Life Sciences, University of Trieste, via Giorgieri 1. 34127 Trieste (Italy).

Supplementary Information
Fig. S1. $^1$H NMR of the methylene protons of the Mosher esters of a) racemic hydroxy ketone 1b and b) enantiomerically pure hydroxyketone (+)-1b obtained by reduction of 3b with *S. Cerevisiae*. 
**Fig. S2.** Scatchard plot of the data from Fig 4b. $r = \frac{[\text{BSA}]_{\text{bound}}}{[\text{BSA}]_{\text{total}}}$; [3b] = molar concentration of free diketone 3b.

Linear fitting ($R = 0.997$) of the data to the equation:

$$\frac{r}{[3b]_{\text{free}} \text{ / M}^{-1}} = \frac{n}{K_d} - \frac{R}{K_d}$$  

(n = number of binding sites)

gives:

$$K_d = \frac{1}{K_d} = (5.2 \pm 0.2) \times 10^4 \text{ M}^{-1}, \quad n/K_d = (5.1 \pm 0.1) \times 10^4 \text{ M}^{-1}.$$
Fig. S3. Superimposition of the IIa binding sites of HSA (green) and BSA (blue) complexed with warfarin. The aminoacids Arg199, Lys222 (BSA) and Lys199, Arg222(HSA) are highlighted. The structure of the HSA complex was obtained from crystallographic data (I. Petitpas, A. A. Bhattacharya, S. Twinet, M. East, S. Curry, J. Biol. Chem., 2001, 276, 22804-22809), and the structure of BSA was obtained by homology modelling.