Albumin-directed stereoselective reduction of 1,3-diketones and β-hydroxyketones to *anti* diols

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Supplementary Information

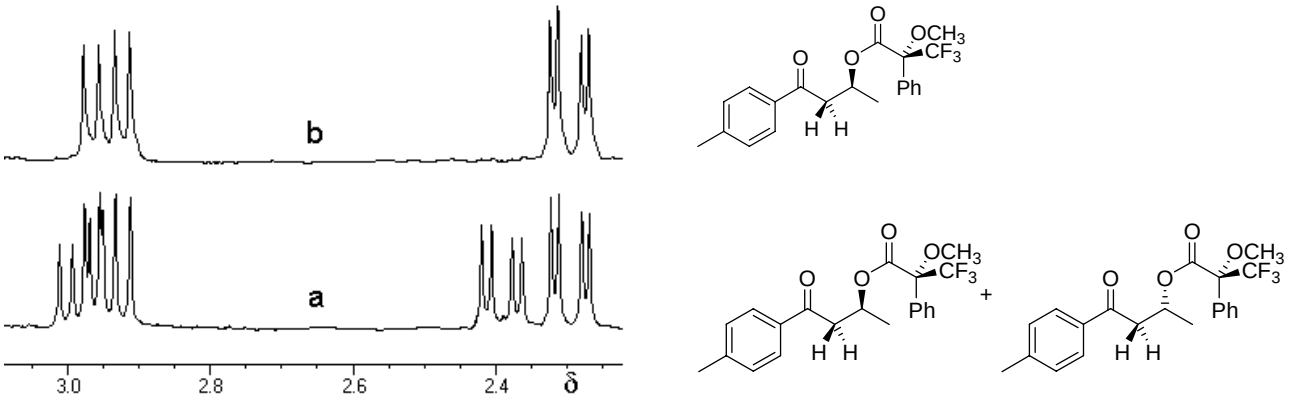

Fig. S1. ^{1}H NMR of the methylene protons of the Mosher esters of a) racemic hydroxy ketone **1b** and b) enantiomerically pure hydroxyketone **(+)-1b** obtained by reduction of 3b with *S. Cerevisiae*.

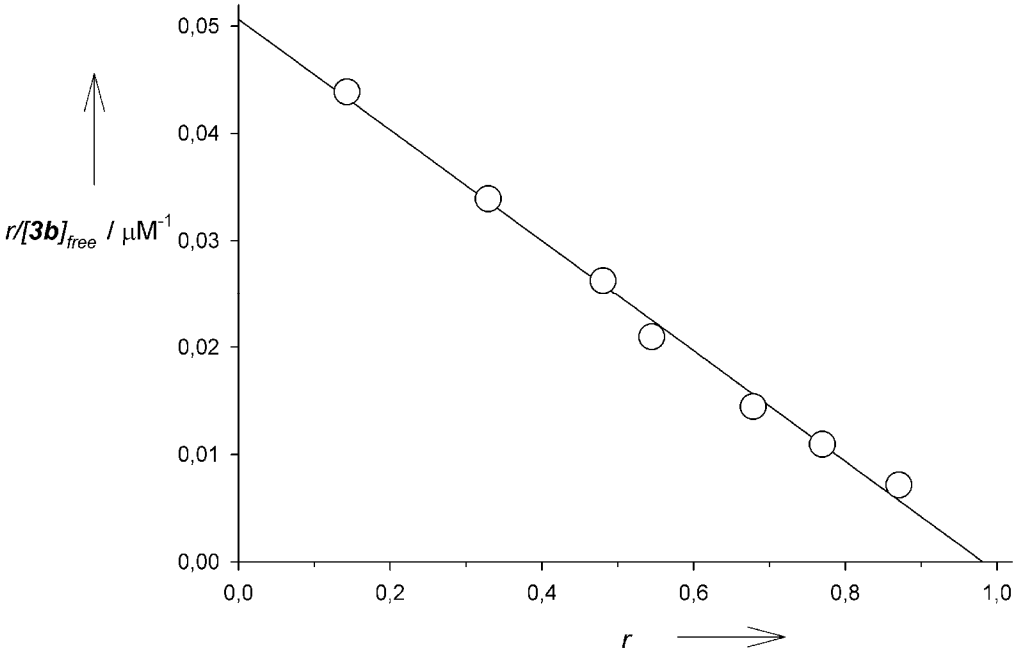

Fig. S2. Scatchard plot of the data from Fig 4b. r = $[BSA]_{bound}/[BSA]_{total}$; [**3b**] = molar concentration of free diketone **3b**.

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

$r/[\mathbf{3b}] = n/K_d - R/K_d$ (n = number of binding sites)

gives:

$K_a=1/K_d=(5.2 \pm 0.2) \times 10^4$ L mol^{-1}, $n/K_d=(5.1 \pm 0.1) \times 10^4$ L mol^{-1}.

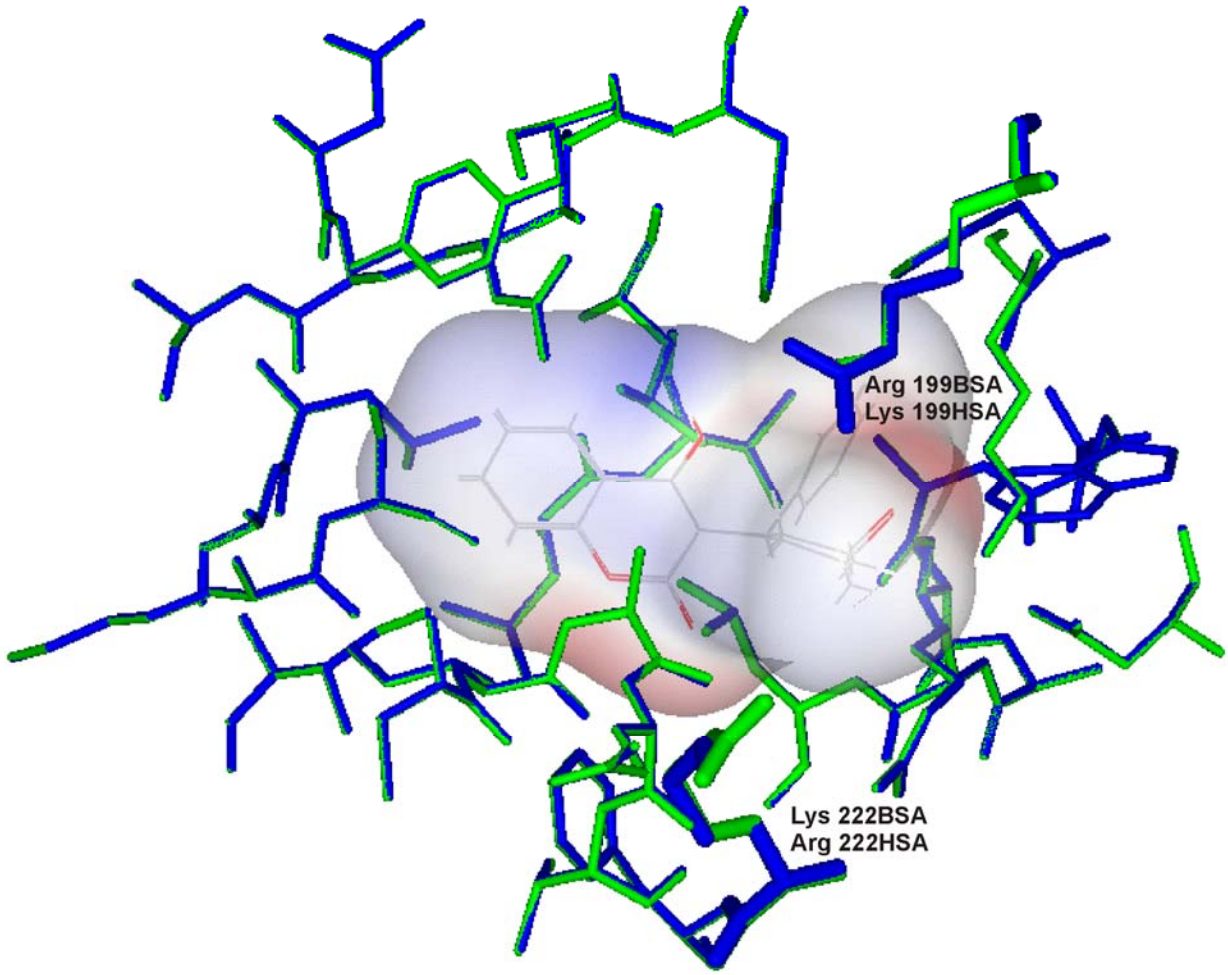

Fig. S3. Superimposition of the IIa binding sites of HSA (green) and BSA (blue) complexed with warfarin. The aminoacids Arg199, Lys222 (BSA) and Lys199, Arg222(HSA) are highlighted. The structure of the HSA complex was obtained from crystallographic data (I. Petitpas, A. A. Bhattacharya, S. Twinet, M. East, S. Curry, J. Biol. Chem., **2001**, *276*, 22804-22809), and the structure of BSA was obtained by homology modelling.