Exploration of Binding Affinities of a 3β,6β-Diacetoxy-5α-cholestan-5-ol with Human Serum Albumin: Insights from Synthesis, Characterization, Crystal Structure, Antioxidant and Molecular docking

Table S1. Crystal data of titled compound

$C_{31}H_{52}O_5$	$F(000) = 1112$
$M_r = 504.72$	$D_x = 1.097$ Mg m^{-3}
Monoclinic, $C2$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 31.634$ (3) Å	Cell parameters from 8643 reflections
$b = 9.9420$ (11) Å	$\theta = 2.2–24.6°$
$c = 9.7325$ (11) Å	$\mu = 0.07$ mm^{-1}
$\beta = 93.568$ (7)°	$T = 293$ K
$V = 3055.0$ (6) Å^3	Plate, colourless
$Z = 4$	0.51 × 0.42 × 0.2 mm

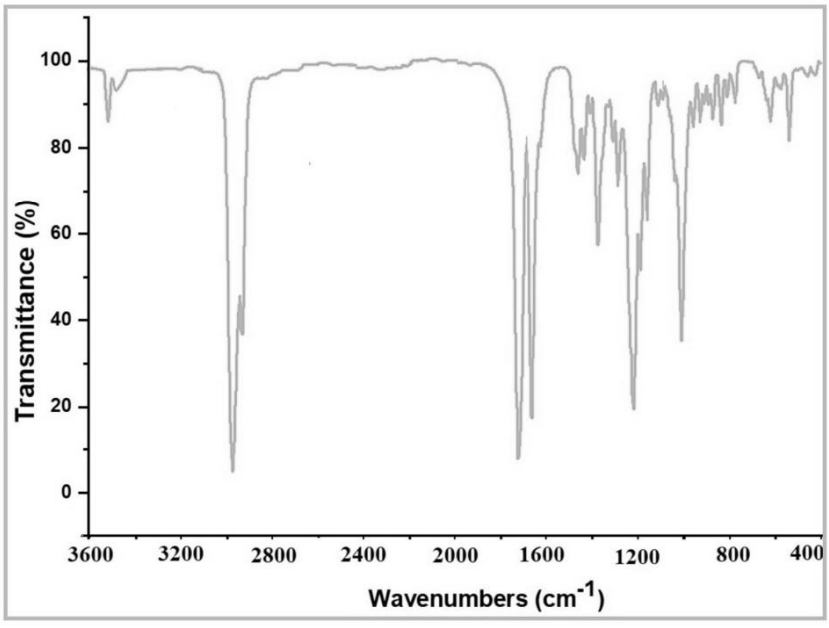

Figure S1. IR spectrum of 3

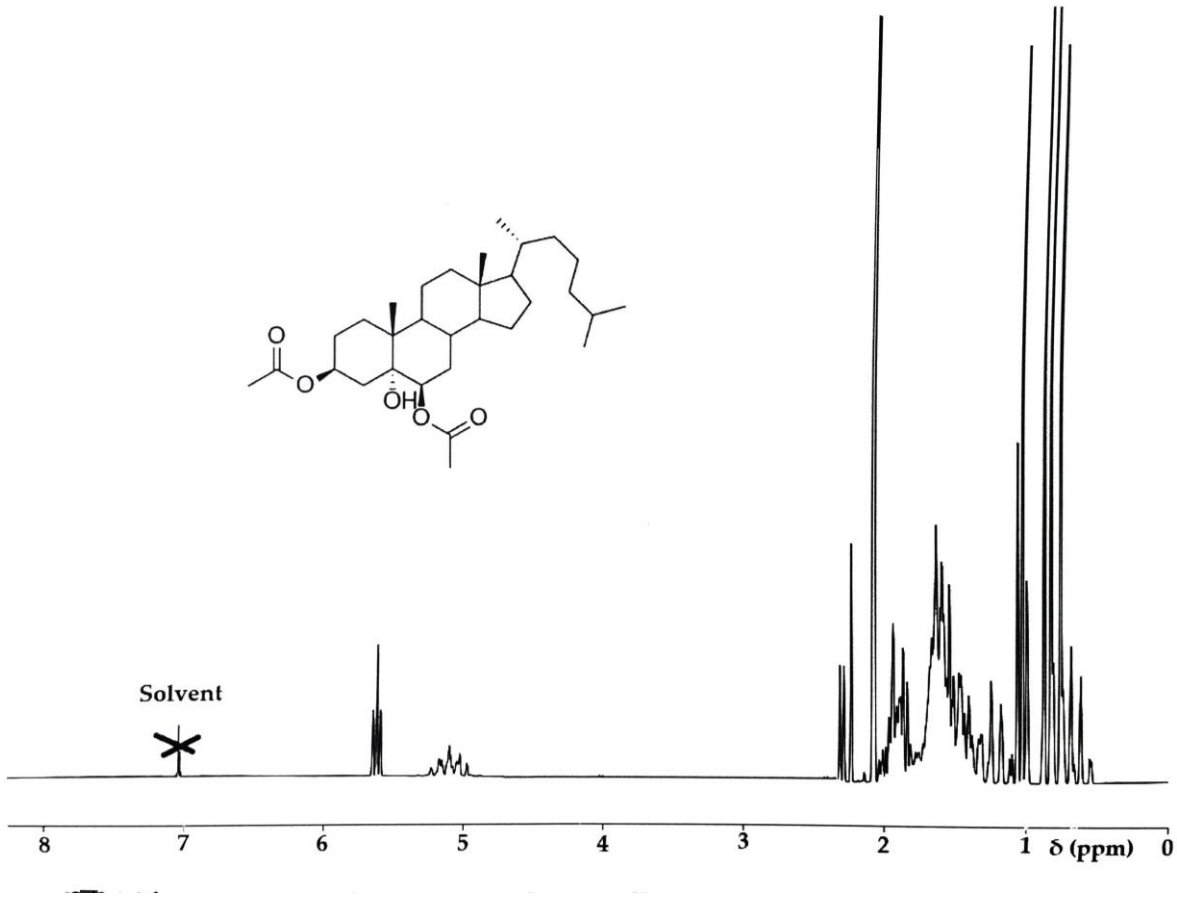

Figure S2. ^{1}H NMR spectrum of 3

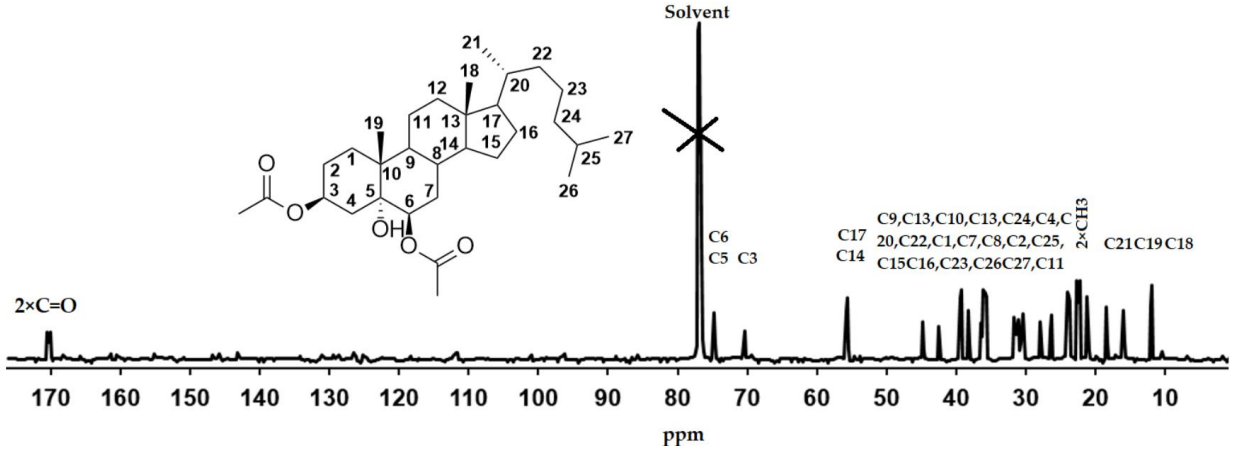

Figure S3. ^{13}C NMR spectrum of 3