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Supplementary Data

Synthesis of 8-hydroxy-2-iminochromene derivatives as selective and potent inhibitors of human carbonyl reductase 1

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Supplementary Table S1.

Nucleotide sequences of the primers used in the construction of the overexpression vector (overexpression) and site-directed mutagenesis (mutagenesis).

Protein	Primer	Sequence (5'……3')
Overexpression [a]		
CBR1	cbr-f	CCCCGAATTCgccacc**ATG**TCGTCCGGCATCC
	cbr-r	CCCCGTCGACTCACCACTGTTCAACT
Mutagenesis [b]		
Met141Gln	M141Q-f	CGTATCTAGCATCCAGAGCGTCAGAGCCC
Met141Val	M141V-f	CGTATCTAGCATCGTGAGCGTCAGAGCCC
Trp229Phe	W229F-f	CTGCTGCCCAGGGTTTGTGAGAACTGACA
Trp229Leu	W229L-f	CTGCTGCCCAGGGTTGGTGAGAACTGACA

[a] The forward primer (cbr-f) contains an *Eco*RI site, Kozak sequence, and start codon, which are shown in underlined, small and bold letters, respectively. The reverse primer (cbr-r) is complementary to the bacterial expression vector containing a *Sal*I site, which is shown in underlined letters. The amplified cDNA was subcloned at the *Eco*RI and *Sal*I sites into the mammalian pGW1 expression vector.

[b] The forward primers used for the site-directed mutagenesis are shown, and the mutated bases are underlined.

Supplementary Fig. S1.

Redocking of cocrystallized ligand Hydroxy-PP. The models obtained from the crystal structure and the redocking are shown in orange and green, respectively.