Target Name	17-beta-HSD
Target TTD ID	TTDR00587

Target Species	Fungus
Chemical Type	Flavonoids
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = (1.75 \times 10^{1} \pm 3.62) \cdot \mathbf{D_1} + (1.51 \times 10^{-1} \pm 3.76 \times 10^{-2}) \cdot \mathbf{D_2} - (4.18 \times 10^{2} \pm 1.42 \times 10^{2}) - (7.41 \times 10^{1} \pm 1.61 \times 10^{1}) \cdot \mathbf{D_4} - (7.42 \times 10^{1} \pm 2.59 \times 10^{1})$ $N = 33,\ r = 0.867,\ F = 21.11,\ s^2 = 0.5073,\ r_{cv}^2 = 0.6302$
QSAR Model 2	$\log(1/IC_{50}) = (2.39 \times 10^{2} \pm 3.54 \times 10^{1}) \cdot \mathbf{D_5} + (1.22 \times 10^{1} \pm 2.85) \cdot \mathbf{D_6} - (2.32 \pm 5.43 \times 10^{-1}) \cdot \mathbf{D_7} + (5.19 \times 10^{1} \pm 1.64) \cdot \mathbf{D_8} - (1.71 \times 10^{2} \pm 5.36 \times 10^{1})$ $N = 30,\ r = 0.885,\ F = 22.79,\ s^2 = 0.3508,\ r_{cv}^2 = 0.6942$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Specification of descriptors used in the derived 4-parameter QSAR models, along with the t test values for all of the descriptors (g—geometrical, q—quantum-chemical descriptors) D5: Max electroph. react. index for an O atom D6: Min. exchange energy for a C–H bond D7: Min. atomic state energy for a C atom D8: Max 1-electron react. index for a C atom
Reference	Flavonoids and cinnamic acid esters as inhibitors of fungal 17β-hydroxysteroid dehydrogenase: A synthesis, QSAR and modelling study. *Bioorganic & Medicinal Chemistry* 14 (2006) 7404–7418

Target Species	Fungus
Chemical Type	Cinnamic acid esters
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = (1.75 \times 10^{1} \pm 3.62) \cdot \mathbf{D_1} + (1.51 \times 10^{-1} \pm 3.76 \times 10^{-2}) \cdot \mathbf{D_2} - (4.18 \times 10^{2} \pm 1.42 \times 10^{2}) - (7.41 \times 10^{1} \pm 1.61 \times 10^{1}) \cdot \mathbf{D_4} - (7.42 \times 10^{1} \pm 2.59 \times 10^{1})$ $N = 33,\ r = 0.867,\ F = 21.11,\ s^2 = 0.5073,\ r_{cv}^2 = 0.6302$
QSAR Model 2	$\log(1/IC_{50}) = (2.39 \times 10^{2} \pm 3.54 \times 10^{1}) \cdot \mathbf{D_5} + (1.22 \times 10^{1} \pm 2.85) \cdot \mathbf{D_6} - (2.32 \pm 5.43 \times 10^{-1}) \cdot \mathbf{D_7} + (5.19 \times 10^{1} \pm 1.64) \cdot \mathbf{D_8} - (1.71 \times 10^{2} \pm 5.36 \times 10^{1})$ $N = 30,\ r = 0.885,\ F = 22.79,\ s^2 = 0.3508,\ r_{cv}^2 = 0.6942$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Specification of descriptors used in the derived 4-parameter QSAR models, along with the t test values for all of the descriptors (g—geometrical, q—quantum-chemical descriptors) D5: Max electroph. react. index for an O atom D6: Min. exchange energy for a C–H bond D7: Min. atomic state energy for a C atom D8: Max 1-electron react. index for a C atom
Reference	Flavonoids and cinnamic acid esters as inhibitors of fungal 17β-hydroxysteroid dehydrogenase: A synthesis, QSAR and modelling study. *Bioorganic & Medicinal Chemistry* 14 (2006) 7404–7418