Target Name	Xanthine oxidase
Target TTD ID	TTDS00056

Target Species	Human
Chemical Type	7-hydroxyflavones
Mode of Action	Inhibitor
QSAR Model 1	$pK_a(\mathrm{F}) = -\log([\mathrm{F}^-]/[\mathrm{F}])\cdot a_{\mathrm{H}}+ = -\log\frac{[A-A_{(\mathrm{F})}]}{[A_{(\mathrm{F}^-)}-A]}\cdot a_{\mathrm{H}}+$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Proton dissociation constants, where A_F and A_{F^-} refers to the absorbances of the flavone in the neutral and anionic forms respectively: A is the absorbance at intermediate pH; au+ is the activity of the hydronium ion. The relative amounts of dissociated and undissociated flavone under the conditions of the enzymatic assay (I = 0.1 M, 25 “C, pH 7.60) were calculated by means of the Henderson-Hasselbath equation.
Reference	A rational approach to the design of flavones as xanthine oxidase inhibitors. *Eur J Med Chem* (1996) 3 1,693-699