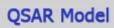
Therapeutic Targets Database





| Target Name | Xanthine oxidase |
|------------------|------------------|
| Target TTD ID | TTDS00056 |

| Target Species | Human |
|-------------------------|--|
| Chemical Type | 7-hydroxyflavones |
| Mode of Action | Inhibitor |
| QSAR Model 1 | $pK_a(F) = -\log ([F]/[F]) \cdot a_H + = -\log \frac{[A - A_{(F)}]}{[A_{(F)} - A]} \cdot a_H +$ |
| Molecular Descriptor | Access the following web-servers to compute molecular descriptors: $\underline{\text{MoDel}}$ and $\underline{\text{e-dragon}}$ 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. <i>Eur J Med Chem</i> (1996) 3 1,693-699 |