Target Name	α-glucosidase
Target TTD ID	TTDC00023

Target Species	Human
Chemical Type	Xanthone derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = 0.239Hs + 0.090S + 0.160N_{\pi} - 1.750$ $n = 34, \quad R^2 = 0.790, \quad Q^2 = 0.733, \quad SD = 0.195, \quad F = 37.524, \quad p < 0.00001$
QSAR Model 2	$\log(1/IC_{50}) = 0.261Hs + 0.122S + 0.152N_{\pi} - 1.758$ $n = 33, \quad R^2 = 0.872, \quad Q^2 = 0.839, \quad SD = 0.154, \quad F = 65.912, \quad p < 0.00001$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Electronic, constitutional, steric, topological, and physicochemical descriptors: LUMO: LUMO energy; HOMO: HOMO energy; E: Total energy; η: Hardness; S: Softness; χ: Electronegativity; ω: Electrophilicity; Dp: Dipole moment; MP: Melting point; BP: Boiling point; Pc: Critical pressure; Tc: Critical temperature; Vc: Critical volume; PMIX: Principal moment of inertia X; PMIY: Principal moment of inertia Y; PMIZ: Principal moment of inertia Z; MR: Molar refractivity; HLC: Henry's law constant; MW: Molecular weight; logP: logP; ClogP: Partition coefficient (octanol water); Hs: Number of H-bonding substituents; N_{π}: number of aromatic rings; HOF: Heat of formation; G: Gibbs energy; Er: Repulsion energy; BIndx: Balaban index; ClsC: Cluster count; Diam: Diameter; TIndx: Molecular topological index; Rad: Radius; ShpA: Shape attribute; ShpC: Shape coefficient; SDe: Sum of degrees; SVDe: Sum of valence degrees; Tcon: Total connectivity; TVCon: Total valence connectivity; Windx: Wiener index. Hs- Number of H-bonding substituents; N_{π} number of aromatic rings; S-Softness

Reference	Synthesis, inhibitory activities, and QSAR study of xanthone derivatives as α-glucosidase inhibitors. *Bioorganic & Medicinal Chemistry* 16 (2008) 7185–7192