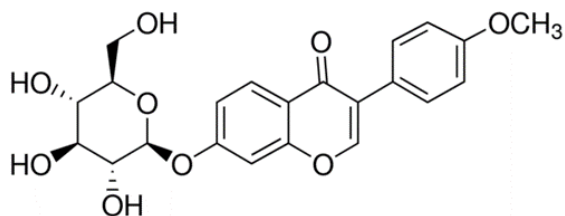


## Supplementar material

The structure of ononin is shown in Figure S1 and the physicochemical properties of ononin and fluconazole are shown in Table S1.

**Figure S1.** Structure of ononin.



**Table S1.** The Physicochemical Properties of Ononin and Fluconazole:

Properties	Ononin	Fluconazole
Formula	C <sub>22</sub> H <sub>22</sub> O <sub>9</sub>	C <sub>13</sub> H <sub>12</sub> F <sub>2</sub> N <sub>6</sub> O
Molecular weight (g/mol)	430.40	306.27
Nº heavy atoms:	31	22
Nº aromatic heavy atoms	16	16
Fraction Csp <sup>3</sup> :	0.32	0.23
Nº rotatable bonds	5	5
Nº H-bond acceptors	9	7
Nº H-bond donors	4	1
Molar Refractivity	108.56	70.71
Topological Polar Surface área (Å <sup>2</sup> )	138.82	81.65