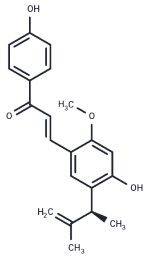
Data Sheet (Cat.No.TN1055)

TargetMol

Licochalcone E

Chemical Properties



CAS No. : 864232-34-8

Formula: C21H22O4

Molecular Weight: 338.4

Storage: Store at low temperature,Keep away from moisture
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Licochalcone E is a potential LXRβ agonist.
Targets(IC50)	Akt,Autophagy,Liver X Receptor,p38 MAPK,PPAR,TNF
In vitro	In this study, the quantitative pharmacophores were constructed by 3D-QSAR pharmacophore (Hypogen) method based on the LXRβ agonists. The optimal pharmacophore model containing one hydrogen bond acceptor, two hydrophobics and one ring aromatic was obtained based on five assessment indictors, including the correlation between predicted value and experimental value of the compounds in training set (correlation), α?cost of the models (α?cost), hit rate of active compounds (HRA), identification of effectiveness index (IEI) and comprehensive evaluation index (CAI). And the values of the five assessment indicators were 0.95, 128.65, 84.44%, 2.58 and 2.18 respectively. The best model as a query to screen the traditional Chinese medicine database (TCMD), a list of 309 compounds was obtained andwere then refined using Libdock program. Finally, based on the screening rules of the Libdock score of initial compound and the key interactions between initial compound and receptor, four compounds, demethoxycurcumin, isolicoflavonol, Licochalcone E and silydianin, were selected as potential LXRβ agonists[1]

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.9551 mL	14.7754 mL	29.5508 mL
5 mM	0.591 mL	2.9551 mL	5.9102 mL
10 mM	0.2955 mL	1.4775 mL	2.9551 mL
50 mM	0.0591 mL	0.2955 mL	0.591 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Discovery of potential LXRβ agonists from Chinese herbs using molecular simulation methods.Zhongguo Zhong Yao Za Zhi. 2016 Aug;41(16):3065-3071.