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# **Data Sheet**

Product Name:	β-Hydroxyisovalerylshikonin	
Cat. No.:	CS-0032419	HO
CAS No.:	7415-78-3	
Molecular Formula:	C <sub>21</sub> H <sub>24</sub> O <sub>7</sub>	ОН
Molecular Weight:	388.41	
Target:	EGFR; Src	$HO_{I} = I = I = I$
Pathway:	JAK/STAT Signaling; Protein Tyrosine Kinase/RTK	
Solubility:	DMSO : 10 mg/mL (25.75 mM; ultrasonic and warming and heat to $60^{\circ}$ C)	

## **BIOLOGICAL ACTIVITY:**

Beta-hydroxyisovalerylshikonin is a natural product isolated from Lithospermum erythrorhizon, acts as a potent inhibitor of **protein tyrosine kinases (PTK)**, with **IC**<sub>50</sub>s of 0.7 $\mu$ M and 1 $\mu$ M for EGFR and v-Src receptor, respectively. Beta-hydroxyisovalerylshikonin is effective against a wide variety of tumor cell lines, and most efficiently induces cell-death in NCI-H522 and DMS114 cells<sup>[1]</sup>. IC50 & Target:IC50: 0.7  $\mu$ M (EGFR), 1  $\mu$ M (v-Src)<sup>[1]</sup>

#### **References:**

[1]. Hashimoto S, et al. Beta-hydroxyisovalerylshikonin is a novel and potent inhibitor of protein tyrosine kinases. Jpn J Cancer Res. 2002 Aug;93(8):944-51.

#### **CAIndexNames:**

Butanoic acid, 3-hydroxy-3-methyl-, (1R)-1-(1,4-dihydro-5,8-dihydroxy-1,4-dioxo-2-naphthalenyl)-4-methyl-3-penten-1-yl ester

### SMILES:

CC(C)(O)CC(O[C@@H](C(C1=O)=CC(C2=C1C(O)=CC=C2O)=O)C/C=C(C)\C)=O

## Caution: Product has not been fully validated for medical applications. For research use only.

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