



Molecular Formula: C₂₁H₂₂O₆
Molecular Weight: 370.401
Accurate Mass: 370.14164
Percentage Composition: C 68.10%; H 5.99%; O 25.92%
Biological Source: Isol. from *Lithospermum erythrospermum*, *Lithospermum euchromum* and *Jatropha glandulifera*
Physical Description: Red prisms or red-violet needles
Melting Point: Mp 113-114°
Optical Rotation: $[\alpha]_{600}^{22} +222$ (EtOH)
UV: [neutral] $\lambda_{\max}$ 275 (); 483 (); 520 (); 560 () (MeOH) (Berdy)
Hazard & Toxicity: **BERDY HAZD : LD₅₀ (mus, ipr) 48 mg/kg**

>>Derivative: O^{I'}-(3,4-Dimethyl-3-pentenoyl)
Synonym(s): Teracrylshikonin

CAS Registry Number: 52438-11-6

Molecular Formula: C₂₃H₂₆O₆
Molecular Weight: 398.455
Accurate Mass: 398.17294
Percentage Composition: C 69.33%; H 6.58%; O 24.09%
Biological Source: Isol. from *Lithospermum euchromum*
Physical Description: Amorph.
Optical Rotation: $[\alpha]_{600}^{17} -92$ (EtOH)

>>Derivative: O^{I'}-(4-Hydroxy-2,4-dimethyl-2-pentenoyl)

CAS Registry Number: 161527-58-8

Molecular Formula: C₂₃H₂₆O₇
Molecular Weight: 414.454
Accurate Mass: 414.167855
Percentage Composition: C 66.65%; H 6.32%; O 27.02%
Biological Source: Isol. from the roots of *Lithospermum erythorhizon*
Other Data: Stereochem. not confirmed

>>Derivative: O^{I'}-Benzoyl
Synonym(s): Benzoylshikonin

Molecular Formula: C₂₃H₂₀O₆
Molecular Weight: 392.407
Accurate Mass: 392.12599
Percentage Composition: C 70.40%; H 5.14%; O 24.46%
Biological Source: Constit. of *Moltkiopsis ciliata*

>>Derivative: O^{I'}-Angeloyl
Synonym(s): Angeloylshikonin

CAS Registry Number: 57094-89-0

Molecular Formula: C₂₁H₂₂O₆
Molecular Weight: 370.401
Accurate Mass: 370.14164
Percentage Composition: C 68.10%; H 5.99%; O 25.92%
Biological Source: Constit. of *Alkanna hirsutissima*
Physical Description: Viscous oil

>>Variant: (S)-form

CAS Registry Number: 517-88-4

Molecular Formula: C₁₆H₁₆O₅
Molecular Weight: 288.299
Accurate Mass: 288.099775
Percentage Composition: C 66.66%; H 5.59%; O 27.75%
Biological Source: Constit. of *Alkanna tinctoria* and *Onosma echoides*. Also from *Lithospermum arvense*, and others
Biological Use/Importance: Antineoplastic agent. Used in the treatment of ulcer oruris
Physical Description: Reddish-bronze needles (Et₂O/EtOH)
Melting Point: Mp 116-117° (149°)
Optical Rotation: $[\alpha]$