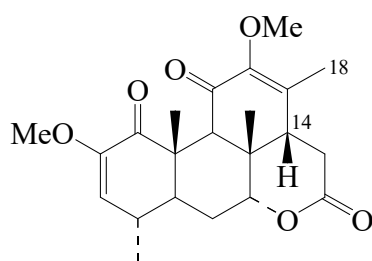




>>Entry Name: Quassin

Synonym(s): Nigakilactone D



CAS Registry Number: 76-78-8

Molecular Formula: C₂₂H₂₈O₆

Molecular Weight: 388.46

Accurate Mass: 388.18859

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Biological Source: Bitter constit. of *Quassia amara*, *Picrasma excelsa* and *Ailanthus glandulosa*

Biological Use/Importance: Shows insecticidal activity. Antiamoebic agent

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 221-222°

Optical Rotation: $[\alpha]_D^{20} +34.5$ (c, 5.09 in CHCl₃)

Calculated Log P Data: Log P 0.5 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 255 (ϵ 11650) (MeOH) (Derep)

>>Derivative: 18-Hydroxy

Synonym(s): 18-Hydroxyquassin

Molecular Formula: C₂₂H₂₈O₇

Molecular Weight: 404.459

Accurate Mass: 404.183505

Percentage Composition: C 65.33%; H 6.98%; O 27.69%

Biological Source: Isol. from coml. Quassin

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 232-233°

Optical Rotation: $[\alpha]_D^{20} +24$ (c, 1 in CHCl₃)

>>Derivative: 14-Epimer

Synonym(s): Isoquassin. Picrasmin

Molecular Formula: C₂₂H₂₈O₆

Molecular Weight: 388.46

Accurate Mass: 388.18859

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Biological Source: Isol. from *Aeschrion excelsa*

Biological Use/Importance: Shows insecticidal activity

Physical Description: Plates and rods (MeOH aq.)

Melting Point: Mp 222-225°

Optical Rotation: $[\alpha]_D^{20} +46.6$ (CHCl₃)

Calculated Log P Data: Log P 0.5 (uncertain value) (calc)

>>Derivative: 1 α -Alcohol, Me ether

Synonym(s): 1 α -O-Methylquassin

Molecular Formula: C₂₃H₃₂O₆

Molecular Weight: 404.502

Accurate Mass: 404.21989

Percentage Composition: C 68.29%; H 7.97%; O 23.73%

Biological Source: Constit. of *Quassia amara*

Physical Description: Powder (MeOH)

Melting Point: Mp 168-172°

References: