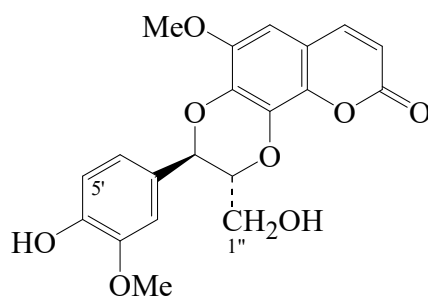




>>Entry Name: Cleomiscosin A

Synonym(s): Cleosandrin



CAS Registry Number: 76948-72-6

Molecular Formula: C₂₀H₁₈O₈

Molecular Weight: 386.357

Accurate Mass: 386.10017

Percentage Composition: C 62.18%; H 4.70%; O 33.13%

Biological Source: Constit. of *Cleome viscosa*, *Soulamea soulameoides*, *Matayba arborescens* and *Cleome icosandra*

Physical Description: Cryst.

Melting Point: Mp 250-252° (247-249°)

Optical Rotation: $[\alpha]_D^{25}$ 0 (c, 0.5 in MeOH)

UV: [neutral] $\lambda_{\max}$ 211 (ε 29500); 232 (ε 25100); 287 (ε 12600); 325 (ε 17800) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 211 (ε 29500); 232 (ε 25100); 233 (ε 28183); 287 (ε 12600); 288 (ε 6920); 325 (ε 17800) (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 288 (ε 5661); 327 (ε 10550) (EtOH) (Berdy)

>>Derivative: 5'-Hydroxy

Synonym(s): 5''-Demethylaquillochin

CAS Registry Number: 305364-91-4

Molecular Formula: C₂₀H₁₈O₉

Molecular Weight: 402.357

Accurate Mass: 402.095085

Percentage Composition: C 59.70%; H 4.51%; O 35.79%

Biological Source: Constit. of *Mallotus apelta*

Physical Description: Needles

Melting Point: Mp 245-246°

>>Derivative: 5'-Methoxy

Synonym(s): Cleomiscosin C. Aquillochin

CAS Registry Number: 84575-10-0

Molecular Formula: C₂₁H₂₀O₉

Molecular Weight: 416.384

Accurate Mass: 416.110735

Percentage Composition: C 60.58%; H 4.84%; O 34.58%

Biological Source: Constit. of *Aquilaria agallocha* and *Cleome viscosa*

Physical Description: Needles (MeOH/EtOAc)

Melting Point: Mp 255°

Optical Rotation: $[\alpha]_D$ 0 (c, 0.08 in MeOH)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. H₂O

UV: [neutral] $\lambda_{\max}$ 232 (ε 25600); 280 (ε 4160); 322 (ε 12160) (MeOH) (Berdy) [base] $\lambda_{\max}$ 258 (); 328 () (MeOH-NAOH) (Berdy)

>>Derivative: 5'-Methoxy, 6-demethoxy

Synonym(s): Daphneticin

CAS Registry Number: 83327-22-4

Molecular Formula: C₂₀H₁₈O₈

Molecular Weight: 386.357

Accurate Mass: 386.10017

Percentage Composition: C 62.18%; H 4.70%; O 33.13%

Biological Source: Constit. of *Daphne tangutica*

Physical Description: Cryst. (MeOH/Me₂CO)

Melting Point: Mp 235-238°

Solubility: BERDY SOL: Sol. MeOH, CHCl₃, toluene; poorly sol. hexane, H₂O

UV: [neutral] $\lambda_{\max}$ 242 (ε 9170); 260 (ε 8892); 317 (ε 11230) (MeOH) (Berdy)