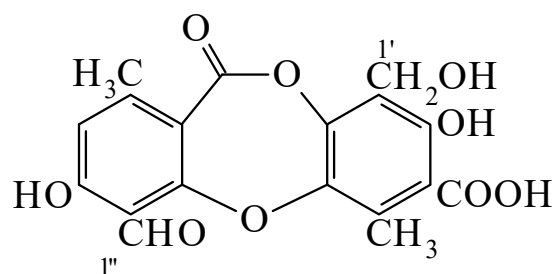




>>Entry Name: Protocetraric acid

Synonym(s): 4-Formyl-3,8-dihydroxy-9-(hydroxymethyl)-1,6-dimethyl-11-oxo-11*H*-dibenzo[*b,e*][1,4]dioxepin-7-carboxylic acid, 9CI



CAS Registry Number: 489-51-0

Molecular Formula: C₁₈H₁₄O₉

Molecular Weight: 374.303

Accurate Mass: 374.063785

Percentage Composition: C 57.76%; H 3.77%; O 38.47%

Biological Source: Isol. from *Oropogon loxensis*, *Ramalina*, *Cetraria*, *Usnea*, *Cladonia*, *Parmelia* and other lichens

Physical Description: Needles

Melting Point: Mp 245-250° (chars, dec. from 220°)

Solubility: BERDY SOL: Poorly sol. H₂O

Other Data: Bitter taste

>>Derivative: Et ester

Synonym(s): Ethyl protocetrarate

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 *Cladonia arbuscula* and *Usnea comosa*

>>Derivative: Mono-Ac

Synonym(s): Monoacetylprotocetraric acid

Molecular Formula: C₂₀H₁₆O₁₀

Molecular Weight: 416.34

Accurate Mass: 416.07435

Percentage Composition: C 57.70%; H 3.87%; O 38.43%

Biological Source: Isol. from *Parmelia* sp.

>>Derivative: 1'-Et ether

Synonym(s): Cetraric acid. Cetrarin

CAS Registry Number: 489-49-6

Molecular Formula: C₂₀H₁₈O₉

Molecular Weight: 402.357

Accurate Mass: 402.095085

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

Biological Source: Artifact formed during isoln. of Protocetraric acid in EtOH medium, formed by pyrolysis of fumaroprotocetraric acid

Physical Description: Prisms

Melting Point: Mp 255° (chars, dec. from 220°)

>>Derivative: 1'-Malonyl

Synonym(s): Malonprotocetraric acid

CAS Registry Number: 64052-98-8

Molecular Formula: C₂₁H₁₆O₁₂

Molecular Weight: 460.35

Accurate Mass: 460.06418

Percentage Composition: C 54.79%; H 3.50%; O 41.71%

Biological Source: Isol. from *Parmotrema conformatum*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 280 dec.°