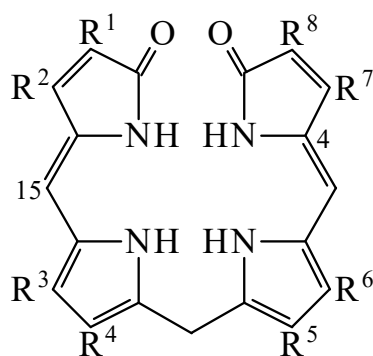




>>Entry Name: Bilirubin

Synonym(s): Bilirubin IX. Haematoidin. Cholerythrin



- IXa $R^1 = R^7 = -CH=CH_2$,
 $R^2 = R^3 = R^6 = R^8 = CH_3$,
 $R^4 = R^5 = -CH_2CH_2COOH$
- IXb $R^1 = R^4 = R^5 = R^7 = CH_3$,
 $R^2 = R^3 = -CH_2CH_2COOH$,
 $R^6 = R^8 = -CH=CH_2$
- IXg $R^1 = R^8 = -CH_2CH_2COOH$,
 $R^2 = R^4 = R^6 = R^7 = CH_3$,
 $R^3 = R^5 = -CH=CH_2$
- IXd $R^1 = R^4 = R^6 = R^8 = CH_2$,
 $R^2 = R^3 = -CH_2CH_2COOH$,
 $R^5 = R^7 = -CH=CH_2$

CAS Registry Number: 635-65-4

Related CAS Registry Numbers(s): 18422-02-1 69853-42-5 69853-43-6 69853-44-7

Molecular Formula: $C_{33}H_{36}N_4O_6$

Molecular Weight: 584.671

Accurate Mass: 584.263486

Percentage Composition: C 67.79%; H 6.21%; N 9.58%; O 16.42%

General Statement: Bilirubin IX α is the ubiquitous isomer and is usually found alone or admixed with IX β . No firm evidence for IX γ and IX δ occurring naturally but this would not be unexpected as the corresponding Biliverdins are known to do so

Biological Source: Pigment from gallstones, blood and urine. Prod. by metab. breakdown of red corpuscles. Ca salt is found in gallstones

Biological Use/Importance: Orange-yellow pigment responsible for jaundice. Prod. in mammals by haem catabolism and transported as an association complex with serum albumin to the liver for glucuronidation and excretion

Physical Description: Orange-brown cryst.

Solubility: Spar. sol. org. solvs.; insol. H_2O

Other Data: X-ray struct. shows internal H-bonding. Photoisomerization gives 4E and/or 15E compds.

Hazard & Toxicity: Exp. reprod. and teratogenic effects. LD₅₀ (mus, orl) >15000 mg/kg

Aldrich: 86179-0

Fluka: 14370

Sigma: B1153

>>Variant: Bilirubin IX α

Synonym(s): 2,17-Diethenyl-1,10,19,22,23,24-hexahydro-3,7,13,18-tetramethyl-1,19-dioxo-21H-biline-8,12-dipropanoic acid, 9CI

>>Derivative: Di-Me ester

CAS Registry Number: 19792-68-8

Molecular Formula: $C_{35}H_{40}N_4O_6$

Molecular Weight: 612.724

Accurate Mass: 612.294786

Percentage Composition: C 68.61%; H 6.58%; N 9.14%; O 15.67%

Physical Description: Orange or red cryst.

Melting Point: Mp 168-169° (dimorph.). Mp 204-205°