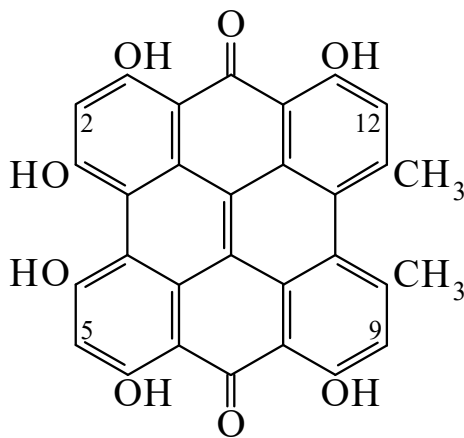




>>Entry Name: Hypericin

Synonym(s): 1,3,4,6,8,13-Hexahydroxy-10,11-dimethylphenanthro[1,10,9,8-*opqra*]perylene-7,14-dione, 9Cl. Mycoporphyrin. Hypericum red



CAS Registry Number: 548-04-9

Molecular Formula: $C_{30}H_{16}O_8$

Molecular Weight: 504.452

Accurate Mass: 504.08452

Percentage Composition: C 71.43%; H 3.20%; O 25.37%

Biological Source: Isol. from the mealy bug *Nipaecoccus aurilanatus*. Widespread in *Hypericum* spp. esp. *Hypericum perforatum* (St. John's wort) which is used as a folk remedy for treating depression and other nervous disturbances

Biological Use/Importance: Antidepressant, tranquilliser; shows potent antiretroviral activity

Physical Description: Solvated blue-black needles

Melting Point: Mp 300° (dec.)

Calculated Log P Data: Log P 4.55 (calc)

UV: [acid] $\lambda_{\max}$ 290 (ϵ 34000); 340 (ϵ 26000); 465 (ϵ 11500); 600 (ϵ 18500); 640 (ϵ 22500) (DMSO as potassium salt) (Derep) [base] $\lambda_{\max}$ 384 (ϵ 12100); 446 (ϵ 12900); 472 (ϵ 13800); 509 (ϵ 10000); 546 (ϵ 24700); 589 (ϵ 43600) (MeOH as potassium salt) (Derep) [neutral] $\lambda_{\max}$ 292 (ϵ 34000); 340 (ϵ 26500); 377 (ϵ 12000); 475 (ϵ 13500); 509 (ϵ 10000); 560 (ϵ 24000); 607 (ϵ 44000) (DMSO) (Derep) [neutral] $\lambda_{\max}$ 508 (); 548 (); 590 () (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 520 (); 559 (); 603 () (Py) (Berdy)

Other Data: Yields cherry-red soln. with red fluor. in org. bases

Fluka: 56690

Sigma: H9252

>>Derivative: Hexabenzoyl

Molecular Formula: $C_{72}H_{40}O_{14}$

Molecular Weight: 1129.1

Percentage Composition: C 76.59%; H 3.57%; O 19.84%

Physical Description: Yellow leaflets

Melting Point: Mp 304-305° (228°)

>>Derivative: 2,5-Dichloro

Synonym(s): 7,7'-Dichlorohypericin

Molecular Formula: $C_{30}H_{14}Cl_2O_8$

Molecular Weight: 573.341

Accurate Mass: 572.006574

Percentage Composition: C 62.85%; H 2.46%; Cl 12.37%; O 22.32%

Biological Source: Constit. of the lichens *Heterodermia obscurata* and *Nephroma laevigatum*

Physical Description: Purple cryst. (AcOH)

Melting Point: Mp 350°

>>Derivative: 2,5,9,12-Tetrachloro

Synonym(s): 2,2',7,7'-Tetrachlorohypericin

Molecular Formula: $C_{30}H_{12}Cl_4O_8$

Molecular Weight: 642.231

Accurate Mass: 639.928628

Percentage Composition: C 56.11%; H 1.88%; Cl 22.08%; O 19.93%

Biological Source: Constit. of *Nephroma laevigatum*

Physical Description: Purple cryst. (AcOH)

Melting Point: Mp 350°