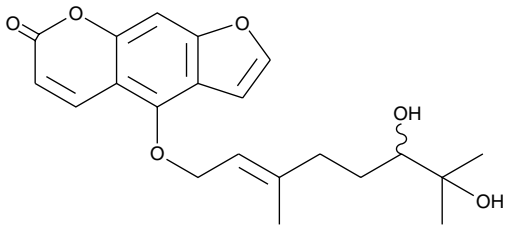
Product Information

6,7-dihydroxy Bergamottin

Item No. 10009598

CAS Registry No.: 145414-76-2
Formal Name: 4-[[(2E)-6,7-dihydroxy-3,7-dimethyl-2-octenyl]oxy]-7H-fuoro[3,2-g][1]benzopyran-7-one
Synonym: 6,7-DHB
MF: $C_{21}H_{24}O_6$
FW: 372.4
Purity: ≥98%
Stability: ≥2 years at -20°C
Supplied as: A crystalline solid
UV/Vis.: λ_{max}: 221, 250, 309 nm



Laboratory Procedures

For long term storage, we suggest that 6,7-dihydroxy bergamottin (6,7-DHB) be stored as supplied at -20°C. It should be stable for at least two years.

6,7-DHB is supplied as a crystalline solid. A stock solution may be made by dissolving the 6,7-DHB in an organic solvent purged with an inert gas. 6,7-DHB is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of 6,7-DHB in ethanol is approximately 10 mg/ml and approximately 30 mg/ml in DMSO and DMF.

6,7-DHB is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, 6,7-DHB should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. 6,7-DHB has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

6,7-DHB is a potent inhibitor of CYP3A4 (IC_{50} = 25 µM).[1] It appears to be the primary compound in grapefruit juice that is responsible for inhibition of testosterone 6β-hydrolase activity. Ingestion of grapefruit juice during treatment regimes with drugs normally metabolized by cytochrome P450 enzymes of the CYP3A subfamily results in a substantial increase in plasma concentration of these agents.[1,2] However, giving a patient grapefruit juice or just 6,7-DHB could be advantageous in cases where a drug is metabolized too quickly by CYP3A4.

References

1. Edwards, D.J., Bellevue, F.H.I., and Woster, P.M. Identification of 6',7'-dihydroxybergamottin, a cytochrome P450 inhibitor, in grapefruit juice. *Drug Metab. Dispos.* **24(12)**, 1287-1290 (1996).
2. Bellevue, F.H.I., Woster, P.M., Edwards, D.J., *et al.* Synthesis and biological evalution of 6',7'-dihydroxybergamottin (6,7-DHB), a naturally occurring inhibitor of cytochrome P450 3A4. *Biooganic & Medicinal Chemistry Letters* **7(20)**, 2593-2598 (1997).

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