# 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
	2-octenyl]oxy]-7H-fuoro[3,2-g][1]	
	benzopyran-7-one	
Synonym:	6,7-DHB	
MF:	$C_{21}H_{24}O_{6}$	ОН ОН
FW:	372.4	
Purity:	≥98%	
Stability:	≥2 years at -20°C	ОН
Supplied as:	A crystalline solid	
UV/Vis.:	$\lambda_{max}$ : 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<sub>50</sub> = 25  $\mu$ M).<sup>1</sup> 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.<sup>1,2</sup> 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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#### SAFETY DATA

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