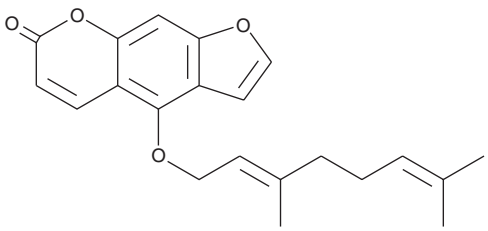
PRODUCT INFORMATION

Bergamottin

Item No. 10009439

CAS Registry No.:	7380-40-7
Formal Name:	4-[[(2E)-3,7-dimethyl-2,6-octadien-1-yl]oxy]-7H-furo[3,2-g][1]benzopyran-7-one
Synonym:	5-Geranoxypsoralen
MF:	$C_{21}H_{22}O_4$
FW:	338.4
Purity:	≥98%
UV/Vis.:	λ_{max}: 250, 308 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

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

Bergamottin is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, bergamottin should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Bergamottin 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.

Description

Bergamottin is a furanocoumarin found in grapefruit juice and lemon, lime, and bergamot oils that has diverse biological activities.[1] *In vitro*, bergamottin inhibits migration and invasion of HT-1080 fibrosarcoma cells at sub-cytotoxic concentrations *via* inhibition of matrix metalloproteinase-9 (MMP-9) expression.[2] It shows antiproliferative activity against HepG2 liver, HL-60 leukemia, and BGC-823 gastric cancer cell lines in a dose-dependent manner and induces cell death of CHO cells following near ultraviolet irradiation.[1,3] Bergamottin inhibits the cytochrome P450 isoform 3A4 (CYP3A4; K_i = 7.7 µM) and is a mixed inhibitor of simvastatin (Item No. 10010344) drug metabolism (K_i = 174 µM).[4,5] It also increases glucose consumption in HepG2 cells in a dose-dependent manner.[6]

References

1. Ashwood-Smith, M.J., Ceska, O., Warrington, P.J., *et al. Photochem. Photobiol.* **55(4)**, 529-532 (1992).
2. Hwang, Y.P., Yun, H.J., Choi, J.H., *et al. Mol. Nutr. Food Res.* **54(7)**, 977-990 (2010).
3. Ashwood-Smith, M.J., Ceska, O., Warrington, P.J., *et al. Photochem. Photobiol.* **55(4)**, 529-532 (1992).
4. Liu, Y., Ren, C., Cao, Y., *et al. Molecules* **22(7)** (2017).
5. He, K., Iyer, K.R., Hayes, R.N., *et al. Chem. Res. Toxicol.* **11(4)**, 252-259 (1998).
6. Le Goff-Klein, N., Koffel, J.C., Jung, L., *et al. Eur. J. Pharm. Sci.* **18(1)**, 31-35 (2003).

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