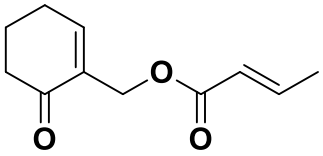
PRODUCT DATA SHEET

COMC

(Cytotoxic)



Synonyms: 2-Crotonyloxymethyl-cyclohex-2-enone

Specifications

Code No.	: 14701
CAS#	: 106281-45-2
Molecular Formula	: $C_{11}H_{14}O_3$
Molecular Weight	: 194.230
Source	:
Supplied as	: Oil
Purity	: > 98% (HPLC)
Long Term Storage	: at -20 °C
Solubility	: Soluble in CH_3CN, $CHCl_3$, DMSO It is recommended to avoid using alcohol such as MeOH or EtOH which may decrease the purity of COMC.

The chemical structure was confirmed by NMR and HRMS.

Application Notes

COMC, synthetic analog of COTC, shows cytotoxic activities against lung cancer cell lines A549 and H460 with the IC_{50} values of 55 and 40 μM, respectively.[1,2] COMC shows 10 times or more potent activity against murine colon adenocarcinoma cell line MAC26 (IC_{50} = 1.1 μM) and human colon adenocarcinoma cell line HCLO (IC_{50} = 1.6 μM) compared to the related natural product, COTC, while COMC and COTC are equitoxic against some other tumor cell lines. [3]

References

1) Glutathionyl transferase catalyzed addition of glutathione to COMC: a new hypothesis for antitumor activity. Hamilton D. S, *et al*. *Org Lett*. 2002 **4**(7) 1209-1212.
2) Arene *cis*-dihydrodiols: Useful precursors for the preparation of analogues of the anti-tumor agent, 2-crotonyloxymethyl-(4*R*,5*R*,6*R*)-4,5,6-trihydroxycyclohex-2-enone (COTC). Arthurs C.L, *et al*. *Bioorg Med Chem Lett*. 2007 **17** 5974-5977.
3) Synthesis and cytotoxicity of shilkimate analogues. Structure: activity studies based on 1-crotonyloxymethyl-3*R*, 4*R*, 5*R*-trihydroxycyclohex-2-enone. Aghil O, *et al. Anti-Cancer Drug Design* 1992 **7** 67-82.