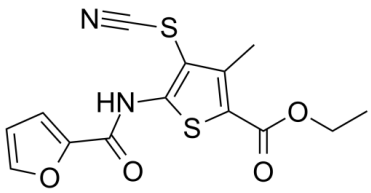
Data Sheet

Product Name:	CBR-5884
Cat. No.:	CS-5648
CAS No.:	681159-27-3
Molecular Formula:	C14H12N2O4S2
Molecular Weight:	336.39
Target:	Others
Pathway:	Others
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 50 mg/mL (148.64 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

CBR-5884 is an active, selective inhibitor of **phosphoglycerate dehydrogenase (PHGDH)** with an IC_{50} of 33 μM. CBR-5884 inhibits de novo **serine synthesis** in cancer cells and is selectively toxic to cancer cell lines with high serine biosynthetic activity. CBR-5884 selectively inhibits the proliferation of melanoma and breast cancer lines that have a high propensity for serine synthesis[1]. IC50 & Target: PHGDH, serine synthesis[1] **In Vitro:** CBR-5884 (15 or 30 μM; 3-5 days) selectively inhibits the proliferation of melanoma and breast cancer lines that have a high propensity for serine synthesis.

PROTOCOL (Extracted from published papers and Only for reference)

Cell assay [1]： Carney cells acclimated to growth in MEM media were plated in a 96-well plate at 6,000 cells per well. The next day, cells were treated with CBR-5884 from 1 μM to 40 μM for 3 h. Drug containing media were then removed, fresh drug-free media added, and cell viability was determined via a CellTiter-Glo or Alamar Blue assay according to the manufacturer's protocol. See SI Methods for details.

References:

[1]. Edouard Mullarky et al. Identification of a small molecule inhibitor of 3-phosphoglycerate dehydrogenase to target serine biosynthesis in cancers Proc Natl Acad Sci U S A, 2016 Feb 16, 113(7):1778-83.

CAIndexNames:

2-Thiophenecarboxylic acid, 5-[(2-furanylcarbonyl)amino]-3-methyl-4-thiocyanato-, ethyl ester

SMILES:

O=C(C1=C(C)C(SC#N)=C(NC(C2=CC=CO2)=O)S1)OCC

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