

## Product Data Sheet

Product Name: CB30865

Cat. No.: GC15207

### Chemical Properties

Cas. No. 206275-15-2

Chemical Name 4-[(7-bromo-2-methyl-4-oxo-1H-quinazolin-6-yl)methyl-prop-2-ynylamino]-N-(pyridin-3-ylmethyl)benzamide

SMILES CC1=NC(=O)C2=CC(=C(C=C2N1)Br)CN(CC#C)C3=CC=C(C=C3)C(=O)NCC4=CN=CC=C4

Formula  $C_{26}H_{22}BrN_5O_2$

M.Wt 516.39

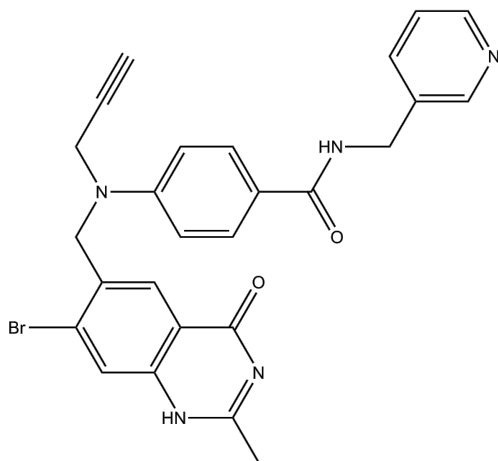
Solubility Soluble in DMSO

Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



### Background

IC50: 2.8 nM for W1L2; 156 nM for isolated mammalian TS

CB30865 is a highly potent cytotoxic agent. The compound inhibits isolated mammalian thymidylate synthase (TS), but this inhibition is insufficient to account for its cellular toxicity. Thymidylate synthase

**Caution: Product has not been fully validated for medical applications. For research use only.**

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(TS) is a critical enzyme in the de novo synthesis of thymidylate (dTTP) and has long been recognized as a target for chemotherapeutic intervention.

In vitro: CB30865 was the most potent growth inhibitory agent (IC<sub>50</sub> values in the range 1–100 nM for several mouse and human cell types). Against W1L2 cells, the analogues of CB300179 and CB300189 demonstrated reduced potency in the presence of exogenous thymidine (dThd), and against a W1L2:C1 TS overproducing cell line. In contrast, CB30865 retained activity in these systems. No cell cycle redistribution was observed following exposure (4–48 h) to an equitoxic concentration of CB30865 [1].

In vivo: The in vivo evaluation of CB30865 was hampered because of its low aqueous solubility (

Clinical trial: No clinical data are available

### References:

- [1] Bavetsias V, Skelton LA, Yafai F, Mitchell F, Wilson SC, Allan B, Jackman AL. The design and synthesis of water-soluble analogues of CB30865, a quinazolin-4-one-based antitumor agent. *J Med Chem.* 2002;45(17):3692-702.
- [2] Skelton LA, Ormerod MG, Titley J, Kimbell R, Brunton LA, Jackman AL. A novel class of lipophilic quinazoline-based folic acid analogues: cytotoxic agents with a folate-independent locus. *Br J Cancer.* 1999;79(11-12):1692-701.

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