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## Product Data Sheet

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Product Name: MBM-55  
Cat. No.: GC36553

### Chemical Properties

Cas. No. 2083622-09-5

SMILES NC(C(C=C1)=C(OCC2=CC=CC(F)=C2)C=C1C3=CN=C4N3C=CC(C5=CN(CCN(C)C)N=C5)=C4)=O

Formula  $C_{28}H_{27}FN_6O_2$  M.Wt 498.55

Solubility Soluble in DMSO Storage Store at -20°C

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

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

Structure

### Background

MBM-55 (compound 42g) is a potent NIMA-related kinase 2 (Nek2) inhibitor with an IC<sub>50</sub> of 1 nM. MBM-55 shows a 20-fold or greater selectivity in most kinases with the exception of RSK1 (IC<sub>50</sub>=5.4 nM) and DYRK1a (IC<sub>50</sub>=6.5 nM). MBM-55 effectively inhibits the proliferation of cancer cells by inducing cell cycle arrest and apoptosis. MBM-55 shows antitumor activities, and no obvious toxicity to mice[1]. IC<sub>50</sub>: 1 nM (Nek2), 5.4 nM (RSK1), 6.5 nM (DYRK1a), 57 nM (CHK1), 91 nM (GSK-3β), 20 nM (ABL), 370 nM (CDK2), 441nM (CDK4), 608 nM (AKT1), 5300 nM (Aurora A)[1]

MBM-55 inhibits MGC-803, HCT-116, Bel-7402 cells proliferation with IC<sub>50</sub>s of 0.53, 0.84, 7.13 μM, respectively[1]. MBM-55 (0.5-1 μM; 24 hours) induces G2/M phase arrest and accumulation of cells with >4N content in HCT-116 cells[1]. MBM-55 (0.5-1 μM; 24 hours) causes cell apoptosis in a concentration-dependent manner in HCT-116 cells[1]. Cell Cycle Analysis[1] Cell Line: HCT-116 cells

MBM-55 (20 mg/kg; i.p.; twice a day for 21 days) exhibits good antitumor activity and a well-tolerated dose schedule in nude mice bearing HCT-116 xenografts[1]. Animal Model: Female BALB/c nu/nu mice (5-6 weeks, bearing HCT-116 xenografts)[1]

[1]. Xi JB, et al. Structure-based design and synthesis of imidazo[1,2-a]pyridine derivatives as novel and potent Nek2 inhibitors with in vitro and in vivo antitumor activities. Eur J Med Chem. 2017 Jan 27;126:1083-1106.

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

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