# Data Sheet

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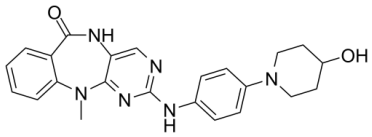
| **Product Name:** | XMD16-5 |
| **Cat. No.:** | CS-6440 |
| **CAS No.:** | 1345098-78-3 |
| **Molecular Formula:** | C23H24N6O2 |
| **Molecular Weight:** | 416.48 |
| **Target:** | Tyrosinase |
| **Pathway:** | Metabolic Enzyme/Protease |
| **Solubility:** | DMSO : ≥ 29 mg/mL (69.63 mM) |



## BIOLOGICAL ACTIVITY:

XMD16-5 is a potent **TNK2** inhibitor with **$IC_{50}$** values of 16 and 77 nM for the D163E and R806Q mutations, respectively. IC50 & Target: IC50: 16 nM (TNK2, D163E mutation), 77 nM (TNK2, R806Q mutation)[1] **In Vitro:** XMD16-5 potently inhibits the growth of the TNK2 mutant expressing cell lines while having little or no effect on the control cells out to the highest tested concentrations (1,000 nM). XMD16-5 has $IC_{50}$s of 16 nM and 77 nM for the D163E and R806Q mutations. The effects of XMD16-5 on TNK2 cell lines are largely due to on-target effects on TNK2. Auto-phosphorylation of overexpressed TNK2 mutants could be blocked with TNK2 inhibitor XMD16-5[1].

## PROTOCOL (Extracted from published papers and Only for reference)

**Kinase Assay:** [1]Kinase targets are tested with biochemical enzymatic kinase assays using the SelectScreen Kinase Profiling Service to determine $IC_{50}$ values. The compounds (XMD16-5) are assayed at 10 concentrations (3-fold serial dilutions starting from 1 μM) at an ATP concentration equal to the ATP Km[1]. **Cell Assay:** [1]Cells are treated with the following inhibitors for 72 hours: dasatinib, AIM-100, XMD8-87 and XMD16-5. Cell viability is measured using a methanethiosulfonate (MTS)-based assay and absorbance (490 nm) is read at 1 and 3 hours after adding reagent[1].

## References:

[1]. Maxson JE, et al. Identification and Characterization of Tyrosine Kinase Nonreceptor 2 Mutations in Leukemia through Integration of Kinase Inhibitor Screening and Genomic Analysis.

## CAIndexNames:

6H-Pyrimido[4,5-b][1,4]benzodiazepin-6-one, 5,11-dihydro-2-[[4-(4-hydroxy-1-piperidinyl)phenyl]amino]-11-methyl-

## SMILES:

O=C1NC2=CN=C(NC3=CC=C(N4CCC(O)CC4)C=C3)N=C2N(C)C5=CC=CC=C15

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

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA