# Data Sheet

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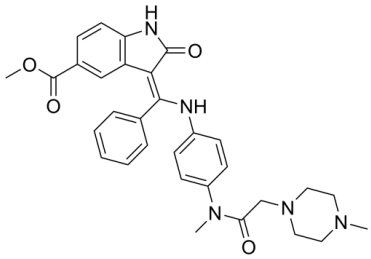
|---|---|
| **Product Name:** | MELK-IN-1 |
| **Cat. No.:** | CS-0021618 |
| **CAS No.:** | 2095596-44-2 |
| **Molecular Formula:** | $C_{31}H_{33}N_5O_4$ |
| **Molecular Weight:** | 539.62 |
| **Target:** | MELK |
| **Pathway:** | PI3K/Akt/mTOR |
| **Solubility:** | 10 mM in DMSO |



## BIOLOGICAL ACTIVITY:

MELK-IN-1 is a potent inhibitor of **maternal embryonic leucine zipper kinase (MELK)** with an $\mathbf{IC_{50}}$ and a $\mathbf{K_i}$ of 3 nM and 0.39 nM, respectively. IC50 & Target: IC50: 3 nM (MELK)

Ki: 0.39 nM (MELK)

[1]

## References:

[1]. Edupuganti R, et al. Discovery of a potent inhibitor of MELK that inhibits expression of the anti-apoptotic protein Mcl-1 and TNBC cell growth. Bioorg Med Chem. 2017 May 1;25(9):2609-2616.

## CAIndexNames:

1H-Indole-5-carboxylic acid, 2,3-dihydro-3-[[[4-[methyl[2-(4-methyl-1-piperazinyl)acetyl]amino]phenyl]amino]phenylmethylene]-2-oxo-, methyl ester, (3Z)-

## SMILES:

O=C(C1=CC2=C(NC(/C2=C(NC3=CC=C(N(C)C(CN4CCN(C)CC4)=O)C=C3)/C5=CC=CC=C5)=O)C=C1)OC



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