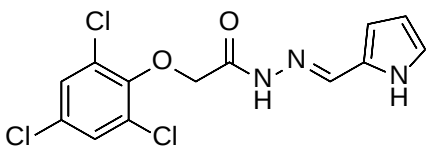
Product data sheet

MedKoo Cat#: 408083 Name: ML239 CAS: 1378872-36-6 Chemical Formula: $C_{13}H_{10}Cl_3N_3O_2$ Exact Mass: 344.9839 Molecular Weight: 346.592	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
ML239 is a potent and selective inhibitor of breast cancer stem cells. ML239 was best-in-class with an IC(50)= 1.18 μM against HMLE_sh_ECad, demonstrated a >23-fold selectivity over the control line, and was toxic to another CSC-like line, HMLE_shTwist, and a breast carcinoma cell line, MDA-MB-231. Gene expression studies conducted with ML239-treated cells showed altered gene expression in the NF-κB pathway in the HMLE_sh_ECad line but not in the isogenic control line.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	53.42	154.11
Ethanol	17.33	50.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.89 mL	14.43 mL	28.85 mL
5 mM	0.58 mL	2.89 mL	5.77 mL
10 mM	0.29 mL	1.44 mL	2.89 mL
50 mM	0.06 mL	0.29 mL	0.58 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Rees MG, Seashore-Ludlow B, Cheah JH, Adams DJ, Price EV, Gill S, Javaid S, Coletti ME, Jones VL, Bodycombe NE, Soule CK, Alexander B, Li A, Montgomery P, Kotz JD, Hon CS, Munoz B, Liefeld T, Dančík V, Haber DA, Clish CB, Bittker JA, Palmer M, Wagner BK, Clemons PA, Shamji AF, Schreiber SL. Correlating chemical sensitivity and basal gene expression reveals mechanism of action. Nat Chem Biol. 2016 Feb;12(2):109-16. doi: 10.1038/nchembio.1986. Epub 2015 Dec 14. PMID: 26656090; PMCID: PMC4718762.

2. Germain AR, Carmody LC, Morgan B, Fernandez C, Forbeck E, Lewis TA, Nag PP, Ting A, VerPlank L, Feng Y, Perez JR, Dandapani S, Palmer M, Lander ES, Gupta PB, Schreiber SL, Munoz B. Identification of a selective small molecule inhibitor of breast cancer stem cells. Bioorg Med Chem Lett. 2012 May 15;22(10):3571-4. doi: 10.1016/j.bmcl.2012.01.035. Epub 2012 Jan 25. PMID: 22503247.

In vivo study

TBD

Product data sheet

7. Bioactivity

Biological target:

ML239 is a potent and selective inhibitor of breast cancer stem cells, with an IC_{50} of 1.16 μM.

In vitro activity

The optimized compound was declared as a probe (ML239) with the NIH Molecular Libraries Program and displayed greater than 20-fold selective inhibition of the breast CSC-like cell line (HMLE_sh_Ecad) over the isogenic control line (HMLE_sh_GFP).

Reference: Bioorg Med Chem Lett. 2012 May 15;22(10):3571-4. https://pubmed.ncbi.nlm.nih.gov/22503247/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.