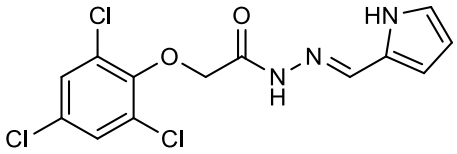
Catalog # 10-1417

ML239

1378872-36-6

(2,4,6-Trichlorophenoxy)-acetic acid (1H-pyrrol-2-ylmethylene)-hydrazide

Lot # X101017



A novel inhibitor of the growth and proliferation of breast cancer stem cells (CSC) discovered in a phenotypic screen employing CSC-like cells produced by inducing human breast epithelial cells into an epithelial-to-mesenchymal transdifferentiated state (HMLE_sh_ECad). ML239 displayed an IC_{50}=1.18 μM against HMLE_sh_ECad and demonstrated a >23-fold selectivity over control cells. It was also toxic to two other CSC-like lines[1,2]. Gene expression studies showed altered gene expression in the NFκB pathway[1] and support activation of fatty acid desaturase 2 (FADS2) as a potential mechanism of action for ML239.[3]

1) Carmody *et al*. (2012), *Phenotypic high-throughput screening elucidates target pathway in breast cancer stem cell-like cells*; J. Biomol. Screening, **17** 1204
2) Germain *et al*. (2012), *Identification of a selective small molecule inhibitor of breast cancer stem cells*; Bioorg. Med. Chem., **22** 3571
3) Rees *et al.* (2015), *Correlating chemical sensitivity and basal gene expression reveals mechanism of action*; Nat. Chem. Biol. **12** 109

PHYSICAL DATA

Molecular Weight:	346.60
Molecular Formula:	$C_{13}H_{10}Cl_3N_3O_2$
Purity:	98% by TLC
	NMR: (Conforms)
Solubility:	DMSO (up to 25 mg/ml), DMF (up to 25 mg/ml), or ethanol (up to 25 mg/ml)
Physical Description:	Beige solid
Storage and Stability:	Store as supplied desiccated at -20°C for up to 2 years from the date of purchase. Solutions in DMSO, DMF or ethanol may be stored at -20°C for up to 3 months.

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