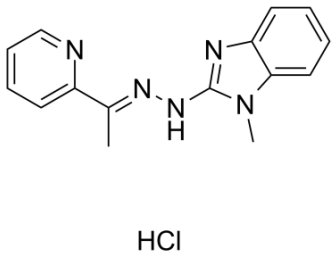
SI-2 hydrochloride

Cat. No.:	HY-101447A
CAS No.:	1992052-49-9
Molecular Formula:	$C_{15}H_{16}ClN_5$
Molecular Weight:	301.77
Target:	Others
Pathway:	Others
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 5 mg/mL (16.57 mM; Need ultrasonic)

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	3.3138 mL	16.5689 mL	33.1378 mL
	5 mM	0.6628 mL	3.3138 mL	6.6276 mL
	10 mM	0.3314 mL	1.6569 mL	3.3138 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

SI-2 (EPH 116 hydrochloride) is a highly promising SRC-3 inhibitor (PPI), with IC_{50} values of 3-20 nM for breast cancer cell death. SI-2 (EPH 116 hydrochloride) has a much improved toxicity and pharmacokinetic profile, with acceptable oral availability[1].

IC_{50} & Target

IC50：3-20 nM (breast cancer cell death)[1].

In Vitro

SI-2 selectively reduce the transcriptional activities and the protein concentrations of SRC-3 in cells through direct physical interactions with SRC-3[1].

SI-2 selectively induces breast cancer cell death with IC_{50} values in the low nanomolar range (3-20 nM), but not affect normal cell viability[1].

SI-2 (100 nM) decreases cell motility, invasion, and tumor metastasis in MDAMB-468 cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1].

Cell Line:	MDA-MB-468 cells.
Concentration:	100 nM.
Incubation Time:	12 hours.
Result:	Significantly reduced the motility of cancer cells.

Western Blot Analysis[1].

Cell Line:	MDAMB-468 cells.
Concentration:	0-200 nM.
Incubation Time:	24 hours.
Result:	Significantly reduced SRC-3 protein levels. Did not decrease the SRC-3 mRNA level.

Western Blot Analysis[1].

Cell Line:	Cancer cells.
Concentration:	0-200 nM.
Incubation Time:	24 hours.
Result:	Caused PARP cleavage.

In Vivo

SI-2 causes minimal acute cardiotoxicity based on a hERG channel blocking assay and an unappreciable chronic toxicity to major organs based on histological analyses[1].
SI-2 is a drug-like molecule and meets all of the criteria of Lipinski's rule[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	MDA-MB-468 breast cancer mouse model[1].
Dosage:	2 mg/kg.
Administration:	Twice daily for 5 weeks (Vehicle, PBS).
Result:	Significantly inhibit tumor growth. SRC-3 levels in SI-2–treated tumor tissues were significantly lower than the PBS treated control group.

Animal Model:	CD1 mice[1].
Dosage:	20 mg/kg (Pharmacokinetic Analysis).
Administration:	Intraperitoneal administration once.
Result:	$T_{1/2}$ = 1 h, C_{max} of 3.0 μM, and the time to reach the maximum plasma concentration t_{max} of 0.25 h. SI-2 only degrades slightly (less than 5%) at pH 1.6 and 3.0 within 6 h, and is stable in buffers with pH ≥ 5.

REFERENCES

[1]. Song X, et al. Development of potent small-molecule inhibitors to drug the undruggable steroid receptor coactivator-3. Proc Natl Acad Sci U S A. 2016 May 3;113(18):4970-5.

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