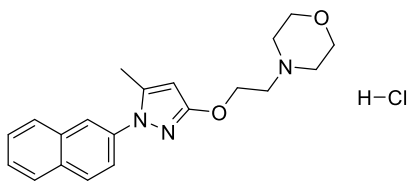
Product data sheet

MedKoo Cat#: 526719 Name: E-52862 HCl CAS#: 1265917-14-3 (HCl) Chemical Formula: $C_{20}H_{24}ClN_3O_2$ Molecular Weight: 373.88	
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:

E-52862, also known as S1RA and MR390, is a selective sigma-1 receptor antagonist, with a reported binding affinity of Ki = 17.0 ± 7.0 nM, selective over the sigma-2 receptor and against a panel of other 170 receptors, enzymes, transporters and ion channels. In preclinical studies, S1RA has demonstrated efficacy in relieving neuropathic pain and pain in other sensitizing conditions, associated with an improvement of the emotional negative state. E-52862 attenuates neuropathic pain of different aetiology in rats.

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	50.5	135.07
DMF	10.0	26.75
DMF:PBS (pH 7.2) (1:5)	0.16	0.43
Water	16.67	44.59

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.67 mL	13.37 mL	26.75 mL
5 mM	0.53 mL	2.67 mL	5.35 mL
10 mM	0.27 mL	1.34 mL	2.67 mL
50 mM	0.05 mL	0.27 mL	0.53 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. Díaz JL, Cuberes R, Berrocal J, Contijoch M, Christmann U, Fernández A, Port A, Holenz J, Buschmann H, Laggner C, Serafini MT, Burgueño J, Zamanillo D, Merlos M, Vela JM, Almansa C. Synthesis and biological evaluation of the 1-arylpyrazole class of σ(1) receptor antagonists: identification of 4-{2-[5-methyl-1-(naphthalen-2-yl)-1H-pyrazol-3-yloxy]ethyl}morpholine (S1RA, E-52862). J Med Chem. 2012 Oct 11;55(19):8211-24. doi: 10.1021/jm3007323. Epub 2012 Jul 27. PMID: 22784008.

In vivo study

1. Sánchez-Blázquez P, Pozo-Rodrigálvarez A, Merlos M, Garzón J. The Sigma-1 Receptor Antagonist, S1RA, Reduces Stroke Damage, Ameliorates Post-Stroke Neurological Deficits and Suppresses the Overexpression of MMP-9. Mol Neurobiol. 2018 Jun;55(6):4940-4951. doi: 10.1007/s12035-017-0697-x. Epub 2017 Aug 5. PMID: 28779350; PMCID: PMC5948242.
2. Gris G, Portillo-Salido E, Aubel B, Darbaky Y, Deseure K, Vela JM, Merlos M, Zamanillo D. The selective sigma-1 receptor antagonist E-52862 attenuates neuropathic pain of different aetiology in rats. Sci Rep. 2016 Apr 18;6:24591. doi: 10.1038/srep24591. PMID: 27087602; PMCID: PMC4834548.

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7. Bioactivity

Biological target:

S1RA hydrochloride (E-52862 hydrochloride) is a potent and selective sigma-1 receptor(σ1R, Ki=17 nM) antagonist.

In vitro activity

The functional activity of compound 28 (E-52862) was evaluated using phenytoin, a low potency allosteric modulator of σ1R that shifts known σ1R agonists to significantly higher affinities (Ki ratios without phenytoin vs with phenytoin of >1), while σ1R antagonists show small or no shift to lower affinity values (Ki ratios without phenytoin vs with phenytoin of ≤1). Compound 28 was shown to be a σ 1R antagonist on account of a small shift to lower affinity being observed when incubated in the presence of phenytoin (Ki(without phenytoin)/Ki(with phenytoin) = 0.8).

Reference: J Med Chem. 2012 Oct 11;55(19):8211-24. https://pubmed.ncbi.nlm.nih.gov/22784008/

In vivo activity

The volumetric analysis of the in vivo MRI data showed that neither surgery nor intracerebroventricular (icv) administration significantly changed the total brain volume (437.9 ± 31.1 and. 456.7 ± 24.8, respectively; sham-operated mice 441.4 ± 26.3 mm^3). However, pMCAO produced severe injury in mice when examined 48 h after ischaemia (Fig. 1a). Injury was mostly apparent in the cerebral cortex, and the infarct volume was estimated as affecting 9.7 ± 1.8% of the total brain volume. No damage was observed in the sham-operated mice. Compared with untreated mice, the administration of S1RA 1 h post-surgery improved stroke outcomes (an approximate 50% reduction in the infarct size to 3.48 ± 0.9% of the total brain volume) after permanent cerebral ischaemia (Fig. 1a).

Reference: Mol Neurobiol. 2018; 55(6): 4940–4951. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5948242/

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.