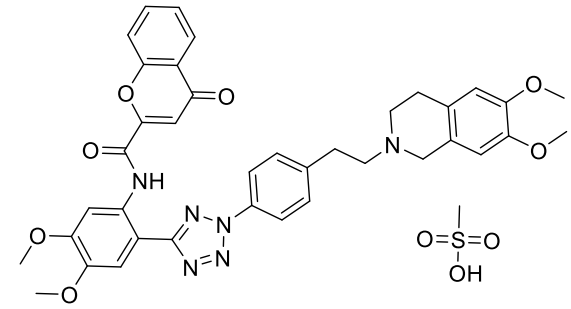
Product data sheet

MedKoo Cat#: 401510 Name: Encequidar mesylate CAS#: 849675-87-2 (mesylate) Chemical Formula: $C_{39}H_{40}N_6O_{10}S$ Exact Mass: 784.2527 Molecular Weight: 784.8410	
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:
Encequidar, also known as HM-30181, is an oral P-glycoprotein (P-gp) inhibitor developed to enhance the oral bioavailability of P-gp substrate drugs. Encequidar showed the highest potency (IC(50)=0.63nM) among several MDR1 inhibitors, including cycloporin A, XR9576, and GF120918, and effectively blocked transepithelial transport of paclitaxel in MDCK monolayers (IC(50)=35.4nM). Encequidar is currently under clinical trials.

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	25.0	31.85

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.27 mL	6.37 mL	12.74 mL
5 mM	0.25 mL	1.27 mL	2.55 mL
10 mM	0.13 mL	0.64 mL	1.27 mL
50 mM	0.03 mL	0.13 mL	0.25 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. Smolinski MP, Urgaonkar S, Pitzonka L, Cutler M, Lee G, Suh KH, Lau JYN. Discovery of Encequidar, First-in-Class Intestine Specific P-glycoprotein Inhibitor. J Med Chem. 2021 Apr 8;64(7):3677-3693. doi: 10.1021/acs.jmedchem.0c01826. Epub 2021 Mar 17. PMID: 33729781.
2. Joo KM, Song SY, Park K, Kim MH, Jin J, Kang BG, Jang MJ, Lee GS, Kim MS, Nam DH. Response of brain specific microenvironment to P-glycoprotein inhibitor: an important factor determining therapeutic effect of P-glycoprotein inhibitor on brain metastatic tumors. Int J Oncol. 2008 Oct;33(4):705-12. PMID: 18813783.

In vivo study

1. Smolinski MP, Urgaonkar S, Pitzonka L, Cutler M, Lee G, Suh KH, Lau JYN. Discovery of Encequidar, First-in-Class Intestine Specific P-glycoprotein Inhibitor. J Med Chem. 2021 Apr 8;64(7):3677-3693. doi: 10.1021/acs.jmedchem.0c01826. Epub 2021 Mar 17. PMID: 33729781.
2. Joo KM, Song SY, Park K, Kim MH, Jin J, Kang BG, Jang MJ, Lee GS, Kim MS, Nam DH. Response of brain specific microenvironment to P-glycoprotein inhibitor: an important factor determining therapeutic effect of P-glycoprotein inhibitor on brain metastatic tumors. Int J Oncol. 2008 Oct;33(4):705-12. PMID: 18813783.

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7. Bioactivity

Biological target:

Encequidar mesylate (HM30181 mesylate; HM30181A mesylate) is a competitive and potent P-glycoprotein inhibitor.

In vitro activity

Based on these data, the IC50 of encequidar for inhibition of P-gp in Caco-2 intestinal cells was determined to be 53 nM, demonstrating that encequidar potently inhibits P-gp and prevents the efflux of paclitaxel from intestinal cells in vitro.

Reference: J Med Chem. 2021 Apr 8;64(7):3677-3693. https://pubmed.ncbi.nlm.nih.gov/33729781/

In vivo activity

40 mg/kg paclitaxel (in combination with 20 mg/kg encequidar) suppressed tumor growth by 94% and induced remission of tumor growth until day 47, an outcome superior to the IV paclitaxel arm included in the study. The results of this study demonstrate the ability of encequidar to inhibit P-gp and facilitate the absorption of paclitaxel to therapeutically effective plasma concentrations in vivo. Clinically, paclitaxel is used to treat many different types of cancers, including breast, lung, and ovarian cancer.

Reference: J Med Chem. 2021 Apr 8;64(7):3677-3693. https://pubmed.ncbi.nlm.nih.gov/33729781/