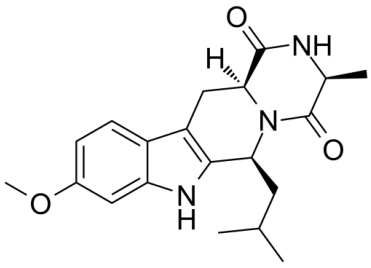
Data Sheet

Product Name:	(S)-ML753286
Cat. No.:	CS-0018774
CAS No.:	1699720-85-8
Molecular Formula:	C20H25N3O3
Molecular Weight:	355.43
Target:	BCRP
Pathway:	Membrane Transporter/Ion Channel
Solubility:	DMSO : ≥ 50 mg/mL (140.67 mM)



BIOLOGICAL ACTIVITY:

(S)-ML753286 is a breast cancer resistance protein (**BCRP**) inhibitor with an **IC_{50}** of 0.6 μM on BCRP efflux transporter. IC50 & Target: IC50: 0.6 μM (BCRP efflux transporter)[1] **In Vivo:** (S)-ML753286 (Compound A) shows the potency and a potent pharmacokinetic (PK) profile in rats (lower clearance [1.54 L/h/kg] and higher bioavailability [123%]). XL388 has moderate terminal elimination half-life with $t_{1/2}$s of 0.9 h and 2.0 h for 2 mg/kg (iv) and 20 mg/kg (po) in rats, respectively[1].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: BCRP-IN-1 (Compound A) is formulated in 0.5% HPMC/0.2% Tween80[1].[1]Mice[1]
To determine pharmacokinetic profile of (S)-ML753286 and Ko143 in vivo, **Sprague-Dawley rats** are administered **2.0 mg/kg or 20 mg/kg (S)-ML753286** or 2.0 mg/kg or 50 mg/kg Ko143, formulated in 0.5% HPMC/0.2% Tween80, via **iv or po**, respectively. After administration of (S)-ML753286 or Ko143, blood is obtained from all animals at predose and at 0.083, 0.25, 0.5, 1, 4, 8, and 24 h postdose. Approximately 200 μL of whole blood is collected from the jugular vein catheter of each animal into tubes containing the anticoagulant dipotassium ethylenediaminetetraacetic acid (K2EDTA) and is further processed into plasma at approximately 4°C[1].

References:

[1]. Li Y, et al. Synthesis of a new inhibitor of breast cancer resistance protein with significantly improved pharmacokinetic profiles. Bioorg Med Chem Lett. 2016 Jan 15;26(2):551-555.

CAIndexNames:

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 2,3,6,7,12,12a-hexahydro-9-methoxy-3-methyl-6-(2-methylpropyl)-, (3S,6S,12aS)-

SMILES:

COC1=CC=C2C(NC3=C2C[C@]4([H])N(C([C@H](C)NC4=O)=O)[C@H]3CC(C)C)=C1

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