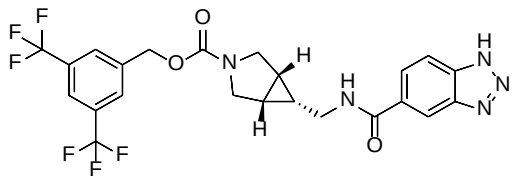
Product data sheet

MedKoo Cat#: 530982 Name: BI-2545 CAS#: 2162961-71-7 Chemical Formula: $C_{23}H_{19}F_6N_5O_3$ Exact Mass: 527.1392 Molecular Weight: 527.43	
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:

BI-2545 is a highly potent, orally active and selective autotaxin inhibitor that significantly reduces LPA levels in vivo. BI-2545 inhibits ATX in the single-digit nanomolar region and translates into good potency in human whole blood. BI-2545 proved to be stable in human and moderately stable in rat liver microsomes. In vitro, BI-2545 showed high Caco-2 permeability and low efflux. BI-2545 shows an excellent PK/target engagement relationship. It is therefore considered a valuable tool for further in vivo studies.

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	250.0	474.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.90 mL	9.48 mL	18.96 mL
5 mM	0.38 mL	1.90 mL	3.79 mL
10 mM	0.19 mL	0.95 mL	1.90 mL
50 mM	0.04 mL	0.19 mL	0.38 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. Kuttruff CA, Ferrara M, Bretschneider T, Hoerer S, Handschuh S, Nosse B, Romig H, Nicklin P, Roth GJ. Discovery of BI-2545: A Novel Autotaxin Inhibitor That Significantly Reduces LPA Levels in Vivo. ACS Med Chem Lett. 2017 Nov 8;8(12):1252-1257. doi: 10.1021/acsmedchemlett.7b00312. PMID: 29259743; PMCID: PMC5733304.

In vivo study

1. Kuttruff CA, Ferrara M, Bretschneider T, Hoerer S, Handschuh S, Nosse B, Romig H, Nicklin P, Roth GJ. Discovery of BI-2545: A Novel Autotaxin Inhibitor That Significantly Reduces LPA Levels in Vivo. ACS Med Chem Lett. 2017 Nov 8;8(12):1252-1257. doi: 10.1021/acsmedchemlett.7b00312. PMID: 29259743; PMCID: PMC5733304.

7. Bioactivity

Biological target:

BI-2545 is a potent autotaxin (ATX) inhibitor that significantly reduces LPA, with IC50s of 2.2 nM and 3.4 nM for human ATX and rat ATX, respectively.

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In vitro activity

In vitro, BI-2545 showed high Caco-2 permeability and low efflux. BI-2545 not only displayed good potency in the LPA and rat whole blood assay but also had favorable ADME properties (see Table 4).

Reference: ACS Med Chem Lett. 2017 Nov 8;8(12):1252-1257. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5733304/

In vivo activity

ATX inhibitor BI-2545 is orally available in rodents, devoid of hERG channel inhibition, and shows an excellent PK/target engagement relationship. Low clearance was observed in vivo in rats, and in vivo oral dosing to rats resulted in good oral exposure. Under these conditions, the sum of the plasma LPA species was reduced up to 90% (see Figure 5), demonstrating high and sustained in vivo efficacy in reducing LPAs.

Reference: ACS Med Chem Lett. 2017 Nov 8;8(12):1252-1257. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5733304/