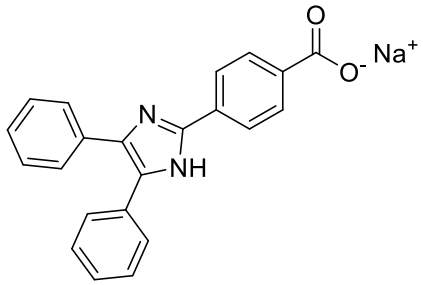
Product data sheet

MedKoo Cat#: 561237 Name: I-XW-053 sodium CAS: 1644644-89-2 Chemical Formula: $C_{22}H_{15}N_2NaO_2$ Molecular Weight: 362.3638	
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:

I-XW-053 sodium inhibits the replication of a diverse panel of primary HIV-1 isolates in PBMCs, while displaying no appreciable cytotoxicity. This antiviral activity is specific to HIV-1, as I-XW-053 displays no effect on the replication of SIV or against a panel of nonretroviruses.

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
TBD	TBD	TBD

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.76 mL	13.80 mL	27.60 mL
5 mM	0.55 mL	2.76 mL	5.52 mL
10 mM	0.28 mL	1.38 mL	2.76 mL
50 mM	0.06 mL	0.28 mL	0.55 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. Kortagere S, Xu JP, Mankowski MK, Ptak RG, Cocklin S. Structure-activity relationships of a novel capsid targeted inhibitor of HIV-1 replication. J Chem Inf Model. 2014 Nov 24;54(11):3080-90. doi: 10.1021/ci500437r. Epub 2014 Oct 28. PMID: 25302989; PMCID: PMC4245176.

2. Kortagere S, Madani N, Mankowski MK, Schön A, Zentner I, Swaminathan G, Princiotto A, Anthony K, Oza A, Sierra LJ, Passic SR, Wang X, Jones DM, Stavale E, Krebs FC, Martín-García J, Freire E, Ptak RG, Sodroski J, Cocklin S, Smith AB 3rd. Inhibiting early-stage events in HIV-1 replication by small-molecule targeting of the HIV-1 capsid. J Virol. 2012 Aug;86(16):8472-81. doi: 10.1128/JVI.05006-11. Epub 2012 May 30. PMID: 22647699; PMCID: PMC3421734.

In vivo study

TBD

7. Bioactivity

Biological target:

I-XW-053 sodium inhibits the replication of a diverse panel of primary HIV-1 isolates in PBMCs.

In vitro activity

Product data sheet

This study has recently designed a novel small molecule inhibitor I-XW-053 using the hybrid structure based method to block the interface between CA N-terminal domains (NTD-NTD interface) with micromolar affinity. In an effort to optimize and improve the efficacy of I-XW-053, this study has developed the structure activity relationship of I-XW-053 compound series using ligand efficiency methods. Compound 34 belonging to subcore-3 showed an 11-fold improvement over I-XW-053 in blocking HIV-1 replication in primary human peripheral blood mononuclear cells (PBMCs).

Reference: J Chem Inf Model. 2014 Nov 24;54(11):3080-90. https://pubmed.ncbi.nlm.nih.gov/25302989/

In vivo activity

TBD

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.