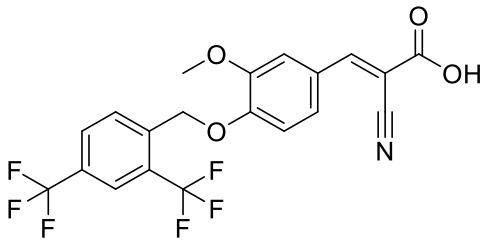
Product data sheet

MedKoo Cat#: 555988 Name: JAN88576 CAS: 2306388-57-6 Chemical Formula: $C_{20}H_{13}F_6NO_4$ Exact Mass: 445.0749 Molecular Weight: 445.3174	
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:
JAN88576, also known as PROTAC ERRα ligand 2, is an estrogen-related receptor α (ERRα) inverse agonist with an IC50 of 5.67 nM. This compound was first reported in ACS Medicinal Chemistry Letters (2019), 10, (5), 767-772. (compound 4a). This product has no formal name at the moment. For the convenience of communication, a temporary code name was therefore proposed according to MedKoo Chemical Nomenclature (see web page: https://www.medkoo.com/page/naming).

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	62.5	140.35

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.25 mL	11.23 mL	22.46 mL
5 mM	0.45 mL	2.25 mL	4.49 mL
10 mM	0.22 mL	1.12 mL	2.25 mL
50 mM	0.05 mL	0.22 mL	0.45 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. Peng L, Zhang Z, Lei C, Li S, Zhang Z, Ren X, Chang Y, Zhang Y, Xu Y, Ding K. Identification of New Small-Molecule Inducers of Estrogen-related Receptor α (ERRα) Degradation. ACS Med Chem Lett. 2019 Apr 12;10(5):767-772. doi: 10.1021/acsmedchemlett.9b00025. PMID: 31097997; PMCID: PMC6512006.

In vivo study

TBD

7. Bioactivity
Biological target:

PROTAC ERRα ligand 2 is an estrogen-related receptor α (ERRα) inverse agonist with an IC_{50} of 5.67 nM. PROTAC ERRα ligand 2 (IC_{50}=5.67 nM) displays a ~11-fold improved potency than XCT790 (IC_{50}=61.3 nM).

In vitro activity

Product data sheet

One of the representative compounds 6c (PROTAC ERRα ligand 2) is capable of specifically degrading ERRα protein by >80% at a relatively low concentration of 30 nM, becoming one of the most potent and selective ERRα degraders to date. Compound 6c could be utilized as a new powerful research tool for further biological investigation of ERRα.

Reference: ACS Med Chem Lett. 2019 Apr 12;10(5):767-772. https://pubmed.ncbi.nlm.nih.gov/31097997/

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.