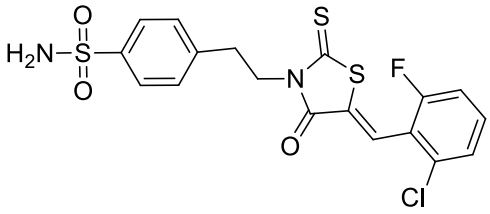
MEINOX

Product Data Sheet v20210303

Product Name **hCA-II inhibitor-3 , hCAIIi-3**

STRUCTURE



Synonyms

hCA-II inhibitor-3 , hCAIIi-3, CA-II inhibitor, carbonic anhydrase inhibitor, Small molecule inhibitor-3 of human carbonic anhydrase-II enzyme

Biological description

Carbonic anhydrase (CA) enzymes are zinc-containing metalloenzymes that maintain pH homeostasis, and they catalyze the CO_2 hydration. hCAs are involved in different physiological as well as pathological processes. In humans, they are divided into 16 isoform forms varying according to tissue distribution and cellular localization (cytosol, membrane, and mitochondria). CA isoforms play a role in a number of biological processes, including acid–base balance control, tumorigenicity, ureagenesis, gluconeogenesis, bone resorption, and calcification. Thus, they are considered a well-established therapeutic target for treatment of a wide range of pathological disorders.

Proprietary tools and expertise in both biology and chemistry were used to develop novel hCA-II inhibitors. In silico, in vitro assays were used to validate small molecule hCA-II inhibitors. The enzyme inhibition activity of newly synthesized compounds on carbonic anhydrase (II) was evaluated. It was found that the IC50 values new molecules were in nanomolar level and much smaller than those of sulfanilamide (reference compound, IC50 of 3.5 μM). hCAIIi-3 was among the most potent carbonic anhydrase (II) inhibitor with the low IC50 value.

Product Information

hCA-II inhibitor-3

- **In silico**: Has a high affinity and preferential binding to Human carbonic anhydrase II enzyme.
- **In vitro**: Inhibits hCA-II enzyme with an IC50 value of 13.8 nM.
- **In vitro**: May inhibit other human CA isoforms.

- **In vivo**: A strong recommendation was also suggested to evaluate these compounds on appropriate in vitro cancer and in vivo animal models to screen most suitable compounds to establish it as future CA (II) inhibitor.

Product Target Proteins / Genes	Carbonic anhydrase (CA) enzymes. Among these, CA I–III, CA VII, and CA XIII are cytosolic enzymes; CA VA and CA VB are located in the mitochondria; CA IV, CA IX, CA XII, and CA XIV are membrane-bounding enzymes; and CA VI takes place in saliva and milk.
Form	Powder
Molecular weight	456.97 g/mol
Solubility Overview	Soluble in DMSO
Inert gas (Yes/No)	Packaged under inert gas
SMILES	S=C3S\C(=C/c1c(F)cccc1Cl)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O
Purity	≥95% by HPLC
Solubility	DMSO (10 mg/ml)
Source	Synthetic
Research areas	Biochemicals, Pharmacology, Signaling, Transcription Factors
Storage	Store at +2°C to +30°C Store under desiccating conditions.

The product can be stored for up to 12 months.

Protect from light.

Do Not Freeze Ok to freeze

Special Instructions Wherever possible, you should prepare and use solutions on the same day. However, if you need to make up stock solutions in advance, we recommend that you store the solution as aliquots in tightly sealed vials at -20°C. Stock solutions are stable for up to 3 months at -20°C. Before use, and prior to opening the vial we recommend that you allow your product to equilibrate to room temperature for at least 1 hour. **Sterility** has not been tested. We recommend filtering working stock solutions with appropriate filters before use in cell culture.

Product Profile & Procedures In order to obtain best results and activity in different techniques and preparations we recommend determining optimal working concentration by dilutions

Precautions This product is for R&D use only, not for drug, household, or other uses. Please consult the Material Safety Data Sheet for information regarding hazards and safe handling practices. Through your purchase, you expressly represent and warrant to MEINOX that you will properly test and use any Products purchased from MEINOX in accordance with industry standards. MEINOX and its authorized distributors reserve the right to refuse to process any order where we reasonably believe that the intended use will fall outside of our acceptable guidelines. Please visit our Terms & Conditions page for more information.

Disclaimer While every effort were made to ensure the accuracy of the information provided in this datasheet, MEINOX will not be liable for any omissions or errors contained herein. MEINOX reserves the right to make changes to this datasheet at any time without prior notice. It is the responsibility of the customer to report product performance issues to MEINOX within 30 days of receipt of the product.

Other Notes Small amounts of compounds may occasionally become entrapped in the seal of the product vial during shipment and storage. If necessary, briefly centrifuge the vial on a tabletop

centrifuge to dislodge any powder in the container`s cap.
Note that this data sheet is not lot-specific and is representative of the current specifications for this product. Please consult the certificate of analysis for further information. Note that shipping conditions may differ from storage conditions.

Bibliography & References

Arif Mermer, Neslihan Demirbas, Ummuhan Cakmak, Ahmet Colak, Ahmet Demirbas, Manikandan Alagumuthu, Sivakumar Arumugam, Discovery of Novel Sulfonamide-Based 5-Arylidenerhodanines as Effective Carbonic Anhydrase (II) Inhibitors: Microwave-Assisted and Ultrasound-Assisted One-Pot Four-Component Synthesis, Molecular Docking, and Anti-CA II Screening Studies, J. Heterocyclic Chem., 56, 2460 (2019), DOI 10.1002/jhet.3635