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IUPAC Name:

Batch No.: 1

Certificate of Analysis

www.tocris.com

Catalog No.: 7890

Product Name: CBMR 0083

CAS Number: 2839486-16-5

1-[3-[[4-Amino-6-[[2-(2,5-dichlorophenyl)ethyl]amino]-1,3,5-triazin-2-yl]methoxy]-5-methylphenyl]-2-pyrrolidinone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage:

Batch Molecular Structure:

 $C_{23}H_{24}Cl_2N_6O_2.$ 487.39 White solid DMSO to 100 mM Store at -20°C

CI CI

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 99.5% purity Consistent with structure Consistent with structure

	Carbon H	ydrogen N	litrogen
Theoretical	56.68	4.96	17.24
Found	57.17	4.79	17

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Print Date: Mar 7th 2024

1

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Description:

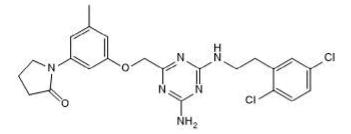
CBMR 0083 is a potent allosteric free fatty acid receptor 1 (FFA1) and 4 (FFA4) agonist (EC₅₀ values are 1 and 2 nM for FFA1 and FFA4, respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{23}H_{24}Cl_2N_6O_2$. Batch Molecular Weight: 487.39 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info: DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

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Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Lückmann et al (2022) Optimization of first-in-class dual-acting FFAR1/FFAR4 allosteric modulators with novel mode of action. ACS Med.Chem.Lett. **13** 1839. PMID: 36518697.

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