# Data Sheet

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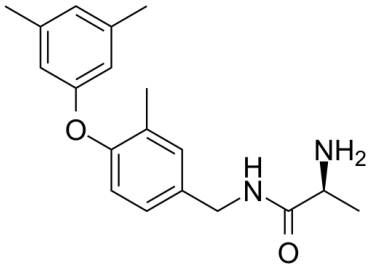
| **Product Name:** | SGC2085 |
| **Cat. No.:** | CS-6152 |
| **CAS No.:** | 1821908-48-8 |
| **Molecular Formula:** | C19H24N2O2 |
| **Molecular Weight:** | 312.41 |
| **Target:** | Histone Methyltransferase |
| **Pathway:** | Epigenetics |
| **Solubility:** | DMSO : ≥ 32 mg/mL (102.43 mM) |



## BIOLOGICAL ACTIVITY:

SGC2085 is a potent and selective coactivator associated arginine methyltransferase 1 (**CARM1**) inhibitor with an **$IC_{50}$** of 50 nM. IC50 & Target: IC50: 50 nM (CARM1)[1] **In Vitro:** SGC2085 which features a methyl at position R1 and a 3,5-dimethylphenoxy at R2 has an $IC_{50}$ of 50 nM for CARM1 and is over 100-fold selective for CARM1 over PRMT6. These results indicate that the presence of a substituent at R1 is essential for potent and selective inhibition of CARM1. With the exception of PRMT6 ($IC_{50}$=5.2 μM), SGC2085 does not inhibit other PRMTs. Considering its small size (MW=312.4 Da), SGC2085 has an excellent selectivity profile, which can probably be further improved by exploiting differences in the binding sites of the two enzymes outside the arginine binding pocket. Compound SGC2085 also shows complete selectivity against a panel of 21 human protein methyltrans- ferases tested at three different concentrations (1,10, and 50 μM). To characterize the mechanism of action of SGC2085 in solution, $IC_{50}$ values are determined at various concentrations of SAM and peptide substrate. Increasing concentration of substrate peptide or cofactor does not affect $IC_{50}$ values, indicative of a noncompetitive mechanism of inhibition, which has been previously shown for other protein methyltransferase inhibitors binding at the substrate pocket[1]. No cellular activity is observed for SGC2085 when tested up to 10 μM (48 h exposure in HEK293 cells), while methylation of BAF155 is abrogated by 10 μM of the dual CARM1/PRMT6 inhibitor MS049. We assume that the absence of cellular activity for SGC2085 is due to poor permeability[1].

## PROTOCOL (Extracted from published papers and Only for reference)

**Cell Assay:** [1]SGC2085 is dissolved in DMSO and diluted with appropriate medium before use. HEK293 cells are grown in 12-well plates in DMEM supplemented with 10% FBS, penicillin (100 U/mL), and streptomycin (100 μg/mL). Thirty percent confluent cells are treated with inhibitors or DMSO. After 48 h, media are removed and cells are lysed in 100 μL of total lysis buffer (20 mM Tris-HCl pH 8.0, 150 mM NaCl, 1 mM EDTA, 10 mM $MgCl_2$, 0.5% Triton X-100, 12.5 U/mL benzonase), complete EDTA-free protease inhibitor cocktail. After 3 min incubation at room temperature, SDS is added to 1% final concentration. Lysates are run on SDS-PAGE, and immunoblotting is done as outlined below to determine the levels of unmethylated and methylated BAF155[1].

## References:

[1]. Ferreira de Freitas R, et al. Discovery of a Potent and Selective Coactivator Associated Arginine Methyltransferase 1 (CARM1) Inhibitor by Virtual Screening. J Med Chem. 2016 Jul 28;59(14):6838-47.

## CAIndexNames:

Propanamide, 2-amino-N-[[4-(3,5-dimethylphenoxy)-3-methylphenyl]methyl]-, (2S)-

## SMILES:

CC1=CC(OC2=CC=C(CNC([C@@H](N)C)=O)C=C2C)=CC(C)=C1

**Caution: Product has not been fully validated for medical applications. For research use only.**

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