



# **Data Sheet**

Product Name: MAC13243
Cat. No.: CS-1183

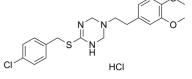
**CAS No.:** 1071638-38-4 **Molecular Formula:** C20H25CI2N3O2S

Molecular Weight: 442.40

Target: Bacterial

Pathway: Anti-infection

Solubility: DMSO: 50 mg/mL (113.02 mM; Need ultrasonic)



#### **BIOLOGICAL ACTIVITY:**

MAC13243, an antibacterial agent, is a likely inhibitor of the bacterial lipoprotein targeting chaperone, LolA. IC50 Value: Target: Antibacterial MAC13243, a molecule that belongs to a new chemical class and that has a unique mechanism and promising activity against multidrug-resistant Pseudomonas aeruginosa. MAC13243 inhibits the function of the LolA protein and represents a new chemical probe of lipoprotein targeting in bacteria with promise as an antibacterial lead with Gram-negative selectivity.

#### References:

- [1]. Barker CA, et al. Degradation of MAC13243 and studies of the interaction of resulting thiourea compounds with the lipoprotein targeting chaperone LoIA. Bioorg Med Chem Lett. 2013 Apr 15;23(8):2426-31.
- [2]. Pathania R, et al. Chemical genomics in Escherichia coli identifies an inhibitor of bacterial lipoprotein targeting. Nat Chem Biol. 2009 Nov;5(11):849-56.

## **CAIndexNames**:

1,3,5-Triazine, 4-[[(4-chlorophenyl)methyl]thio]-1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,6-tetrahydro-, hydrochloride (1:1)

### SMILES:

 $\mathsf{CIC1} = \mathsf{CC} = \mathsf{C}(\mathsf{CSC2} = \mathsf{NCN}(\mathsf{CCC3} = \mathsf{CC}(\mathsf{OC}) = \mathsf{C}(\mathsf{OC})\mathsf{C} = \mathsf{C3})\mathsf{CN2})\mathsf{C} = \mathsf{C1}.\mathsf{C1}$ 

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

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Page 1 of 1 www.ChemScene.com