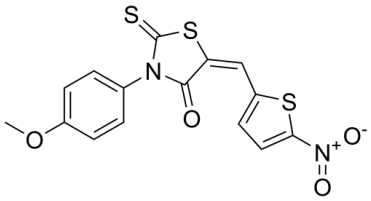
Data Sheet

Product Name:	CCF642
Cat. No.:	CS-5782
CAS No.:	346640-08-2
Molecular Formula:	$C_{15}H_{10}N_2O_4S_3$
Molecular Weight:	378.45
Target:	Apoptosis; PDI
Pathway:	Apoptosis; Cell Cycle/DNA Damage; Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 30 mg/mL



BIOLOGICAL ACTIVITY:

CCF642 is a potent **protein disulfide isomerases (PDI)** inhibitor with an **IC_{50}** of 2.9 μM. CCF642 causes acute endoplasmic reticulum (ER) stress in multiple myeloma cells accompanied by apoptosis-inducing calcium release. CCF642 has broad anti-multiple myeloma activity[1]. IC50 & Target: IC50: 2.9 μM (PDI)[1] ***In Vitro:*** CCF642 (3 μM; 0.5-6 hours) increases PERK dimerization by phosphorylation and IRE1-α oligomerization within 30 minutes in KMS-12-PE confirming accumulation of misfolded ER proteins[1]. CCF642, a bone marrow-sparing compound, exhibits a submicromolar IC_{50} in 10 of 10 multiple myeloma cell lines (MM1.S, MM1.R, KMS-12-PE, KMS-12-BM, NCI-H929, U266, RPMI 8226, JJN-3, HRMM.09-luc, 5TGM1-luc)[1].
In Vivo: CCF642 (10 mg/kg; i.p.; three times a week; for 24 days) significantly prolongs life of 5TGM1-luc-bearing mice and suppresses 5TGM1-luc growth as determined by life imaging[1].

References:

[1]. Vatolin S et al. Novel Protein Disulfide Isomerase Inhibitor with Anticancer Activity in Multiple Myeloma. Cancer Res. 2016 Jun 1;76(11):3340-50.

CAIndexNames:

4-Thiazolidinone, 3-(4-methoxyphenyl)-5-[(5-nitro-2-thienyl)methylene]-2-thioxo-

SMILES:

O=C1N(C2=CC=C(OC)C=C2)C(S/C1=C/C3=CC=C([N+]([O-])=O)S3)=S

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