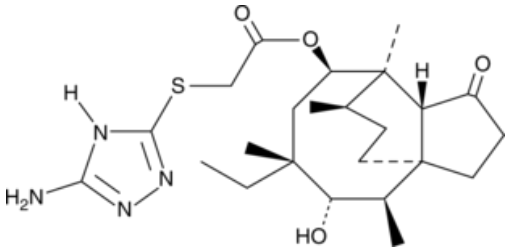
Product Data Sheet

Product Name: Azamulin
Cat. No.: GC42888

Chemical Properties

Cas. No.	76530-44-4		
Chemical Name	(3aS,4R,5S,6R,8R,9R,9aR,10R)-6-ethyldecahydro-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-3a,9-propano-3aH-cyclopentacycloocten-8-yl ester 2-[(3-amino-1H-1,2,4-triazol-5-yl)thio]-acetic acid		
SMILES	O=C1CC[C@@]23[C@@H](C)[C@H](O)[C@@](CC)(C)C[C@@H](OC(CSC4=NN=C(N)N4)=O)[C@](C)([C@H](C)CC3)[C@@]21[H]		
Formula	C24H38N4O4S	M.Wt	478.7
Solubility	20mg/mL in ethanol, or in DMSO, or in DMF	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure			

Background

Azamulin is a selective, irreversible inhibitor of cytochrome P450 (CYP) 3A isoforms (IC50 values range from 26 to 240 nM for CYP3A4 and CYP3A4/5 from different sources). [1] It is at least 50-fold

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less potent against CYP2J2 and 100-fold less effective against all other CYP isoforms. [1] Azamulin potently blocks the hydroxylation of testosterone and midazolam by CYP3A4.[2]

Reference:

[1]. Stresser, D.M., Broudy, M.I., Ho, T., et al. Highly selective inhibition of human CYP3Aa in vitro by azamulin and evidence that inhibition is irreversible. Drug Metabolism and Disposition 32(1), 105-112 (2004).
[2]. Lim, H.K., Duczak, N., Jr., Brougham, K., et al. Automated screening with confirmation of mechanism-based inactivation of CYP3A4, CYP2C9, CYP2C19, CYP2D6, and CYP1A2 in pooled human liver microsomes. Drug Metabolism and Disposition 33(8), 1211-1219 (2005).

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