Product Data Sheet

Product Name: Ro 26-4550 trifluoroacetate
Cat. No.: GC12565

Chemical Properties

Cas. No.	1217448-66-2		
Chemical Name	(S)-methyl 2-(2-((R)-1-carbamimidoylpiperidin-3-yl)acetamido)-3-(4-(phenylethynyl)phenyl)propanoate 2,2,2-trifluoroacetate		
SMILES	OC(C(F)(F)F)=O.NC(N1CCC[C@H](CC(N[C@H](C(OC)=O)CC2=CC=C(C#CC3=CC=CC=C3)C=C2)=O)C1)=N		
Formula	$C_{26}H_{30}N_4O_3.CF_3CO_2H$	M.Wt	560.57
Solubility	<28.03mg/ml in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	Ro 26-4550 trifluoroacetate		

Background

IC50: 3 μM

Ro 26-4550 trifluoroacetate is a competitive reversible inhibitor of interleukin-2 (IL-2) binding to its receptor [1].

Interleukin-2 (IL-2) (a 15.5 kDa cytokine) plays a predominant role in the growth of activated T cells. IL-2 induces T-cell proliferation followed by binding on the T-cell surface with picomolar affinity to a heterotrimeric receptor complex (consisting of R, , and chains). It has proven clinically effective as immunosuppressive agents that antibodies recognize the R receptor subunit (IL-2RR) and discrupte IL-2 binding. Small molecules are capable of preventing the IL-2/IL-2RR interaction as potential orally active successors to the antibody drugs [1].

In vitro: The region of IL-2 perturbed by association with Ro 26-4550 was shown to be

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involved in the binding to IL-2RR. This suggests that Ro 26-4550 competes with IL-2RR for its binding site on IL-2 to interfer with IL-2/IL-2RR binding. [1] .

Analyses of the X-ray structure of Ro 26-4550 binding at the “hot spot” of IL-2 showed that the protein is changeable and then undergo significant rearrangements to create the small molecule binding site. This observation refutes the perception that protein-protein interactions are flat and featureless and indicates that the surface of IL-2 could exist additional nonobvious binding sites (binding a small molecule with high affinity). However, accurate structure-based predictions will be more difficult because of the adaptive nature of the site [2].

In vivo: So far, no study in vivo has been conducted.

Clinical trial: So far, no clinical study has been conducted.

References:
[1]. Tilley JW, Chen L, Fry DC, Emerson SD, Powers GD, Biondi D, Varnell T, Trilles R, Guthrie R, Mennona F, Kaplan G, LeMahieu RA, Carson M, Han R-J, Liu C-M, Palermo R, Ju G. Identification of a small molecule inhibitor of the IL-2/IL-2Rr receptor interaction which binds to IL-2. J. Am. Chem. Soc. 1997, 119, 7589-7590
[2] Braisted AC, Oslob JD, Delano WL, Hyde J, McDowell RS, Waal N, Yu C, Arkin MR, Raimundo BC. Discovery of a potent small molecule IL-2 inhibitor through fragment assembly. J Am Chem Soc. 2003 Apr 2;125(13):3714-5.