Product Data Sheet

Product Name: ONX 0801 trisodium
Cat. No.: GC61159

Chemical Properties

Cas. No.	1097638-00-0		
SMILES	O=C(N[C@H](C(O[Na])=O)CCC(N[C@@H](C(O[Na])=O)CCC(O[Na])=O)=O)C1=CC=C(N([C@H]2CCC3=C2C=C4C(NC(CO)=NC4=O)=C3)CC#C)C=C1		
Formula	$C_{32}H_{30}N_5Na_3O_{10}$	M.Wt	713.58
Solubility		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	ONX 0801 trisodium		

Background

ONX 0801 (BGC 945) trisodium is a thymidylate synthase (TS) inhibitor, targeted to α-folate receptor-overexpressing tumors[1][2].

ONX 0801 (BGC 945) is designed to further reduce toxicity by more effectively targeting cancer cells that overexpress the α-FR[1].ONX 0801 (BGC 945) exhibits IC50 values of of 6.6 μM, 1.1 nM, 3.3 nM, 90 nM and 0.32 μM in A431, A431-FBP, KB, IGROV-1 and JEG-3 cells[2].

BGC 945 (100 mg/kg, ip/iv injection) in the tumor had a longer half-life (28 hours) compared with other tissues[2].BGC 945 (100 mg/kg daily for 16 days) does not lead to body weight loss, macroscopic signs of toxicity to the major organs, or a change in renal function[2].BGC 945 at 100mg/kg induces a 5-20-fold increase in tumor dUrd at 4-72h without increases in the plasma, consistent with tumor targeting[2]. Animal Model: Mice (on the folate-free diet for 5 days were transplanted with tumor and the implants)[2].

[1]. Anna Tochowicz, et al. Development and binding mode assessment of N-[4-[2-propyn-1-yl[(6S)-4,6,7,8-tetrahydro-2-(hydroxymethyl)-4-oxo-3H-cyclopenta[g]quinazolin-6-yl]amino]benzoyl]-l-γ-glutamyl-D-glutamic acid (BGC 945), a novel thymidylate synthase inhibitor that targets tumor cells. J Med Chem. 2013 Jul 11;56(13):5446-55. [2]. David D Gibbs, et al. BGC 945, a novel tumor-selective thymidylate synthase inhibitor targeted to alpha-folate receptor-overexpressing tumors. Cancer Res. 2005 Dec 15;65(24):11721-8. [3]. Chau Ng, et al. Efficacy and tolerability of the thymidylate synthase (TS) inhibitor, BGC 945 is mediated through its selective uptake via the α-folate receptor (α-FR) in IGROV-1 human tumor xenografts. AACR Annual Meeting-- Apr 12-16, 2008; San Diego, CA.

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