CD BioGlyco

SUITE 201, 17 Ramsey Road, Shirley, NY 11967, USA

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Product Information

CCR inhibitor Cenicriviroc, Purity ≥98%

Cat. No.: X23-10-ZQ589

Size: 10 mg; 25 mg; 50 mg; 100 mg

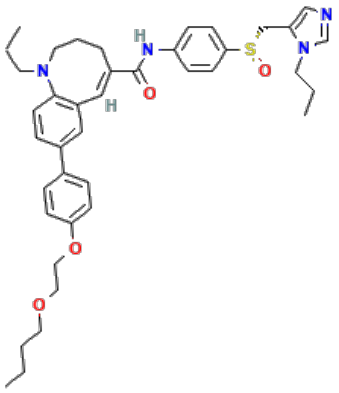
MDL: MFCD28502076

CAS Number: 497223-25-3

Compound CID: 11285792

Synonym: Cenicriviroc; 497223-25-3; TBR-652; TAK-652; TBR652; TBR 652; 15C116UA4Y; CCR inhibitor

This product is for research use only and is not intended for diagnostic use.



Product Information

Description	Cenicriviroc, soluble in DMSO and ethanol and insoluble in water, specifically binds to chemokine receptors. This binding blocks the receptors and prevents the corresponding chemokines from exerting their effects on immune cells, leading to reduced chemotaxis and cell activation.
Molecular Weight	696.94
Molecular Formula	$C_{41}H_{52}N_4O_4S$
IUPAC Name	(5*E*)-8-[4-(2-Butoxyethoxy)phenyl]-1-(2-methylpropyl)-*N*-[4-[(S)-(3-propylimidazol-4-yl)methylsulfinyl]phenyl]-3,4-dihydro-2*H*-1-benzazocine-5-carboxamide
InChI	InChI=1S/C41H52N4O4S/c1-5-7-22-48-23-24-49-38-15-10-32(11-16-38)33-12-19-40-35(25-33)26-34(9-8-21-44(40)28-31(3)4)41(46)43-36-13-17-39(18-14-36)50(47)29-37-27-42-30-45(37)20-6-2/h10-19,25-27,30-31H,5-9,20-24,28-29H2,1-4H3,(H,43,46)/b34-26+/t50-/m0/s1
InChI Key	PNDKCRDVVKJPKG-WHERJAGFSA-N
Canonical SMILES	CCCCOCCOC1=CC=C(C=C1)C2=CC3=C(C=C2)N(CCCC(=C3)C(=O)NC4=CC=C(C=C4)S(=O)CC5=CN=CN5CCC)CC(C)C
Isomeric SMILES	CCCCOCCOC1=CC=C(C=C1)C2=CC/3=C(C=C2)N(CCC/C(=C3)/C(=O)NC4=CC=C(C=C4)[S@@](=O)CC5=CN=CN5CCC)CC(C)C
Form	Lyophilized powder
Purity	≥98%
Solubility	DMSO: 94 mg/mL (134.87 mM); Water: Insoluble; Ethanol: 94 mg/mL (134.87 mM)
Identity	Confirmed by NMR/HPLC/MS.

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Stability	The product is stable for three years when stored at the recommended temperature in lyophilized powder.
Applications	Cenicriviroc can be leveraged to explore its dual antagonist activity on CCR2 and CCR5 in models of nonalcoholic steatohepatitis (NASH) and fibrosis.
Storage	Store at -20ºC.