

Product Information

CCR antagonist Vicriviroc malate, Purity $\geq 98\%$

Cat. No.: X23-10-ZQ515

Size: 5 mg; 10 mg; 25 mg; 50 mg; 100 mg

CAS Number: 541503-81-5

Compound CID: 10218922

Synonym: Vicriviroc Malate; 541503-81-5;

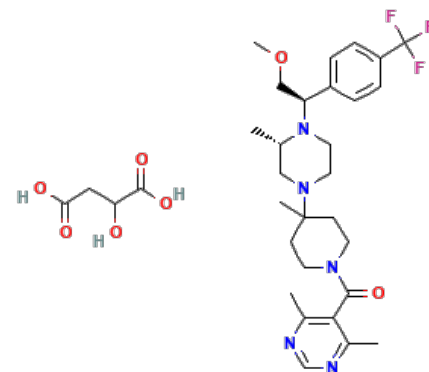
1-[(4,6-Dimethyl-5-pyrimidinyl)carbonyl]-

4-[(3S)-4-[(1R

)-2-methoxy-1-[4-(trifluoromethyl)phenyl]ethyl]-3-methyl-1-piperazinyl]-4-methylpiperidi

ne malate; Vicriviroc (Malate); CCR antagonist

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



Product Information

Description	Vicriviroc malate, soluble in DMSO, water and ethanol, is an active small molecule compound that mediates the CCR signaling pathway.
Molecular Weight	667.7
Molecular Formula	C ₂₈ H ₃₈ F ₃ N ₅ O ₂ ·C ₄ H ₆ O ₅
IUPAC Name	(4,6-Dimethylpyrimidin-5-yl)-[4-[(3S)-4-[(1R)-2-methoxy-1-[4-(trifluoromethyl)phenyl]ethyl]-3-methylpiperazin-1-yl]-4-methylpiperidin-1-yl]methanone;2-hydroxybutanedioic acid
InChI	InChI=1S/C28H38F3N5O2.C4H6O5/c1-19-16-35(14-15-36(19)24(17-38-5)22-6-8-23(9-7-22)28(29,30)31)27(4)10-12-34(13-11-27)26(37)25-20(2)32-18-33-21(25)3;5-2(4(8)9)1-3(6)7/h6-9,18-19,24H,10-17H2,1-5H3;2,5H,1H2,(H,6,7)(H,8,9)/t19-,24-;/m0./s1
InChI Key	HQJIGHNTRUUVLT-RIAYWLAYSAN
Canonical SMILES	CC1CN(CCN1C(COC)C2=CC=C(C=C2)C(F)(F)F)C3(CCN(CC3)C(=O)C4=C(N=CN=C4C)C)C.C(C(C(=O)O)O)C(=O)O
Isomeric SMILES	C[C@H]1CN(CCN1[C@@H](COC)C2=CC=C(C=C2)C(F)(F)F)C3(CCN(CC3)C(=O)C4=C(N=CN=C4C)C)C.C(C(C(=O)O)O)C(=O)O
Form	Lyophilized powder
Purity	$\geq 98\%$
Solubility	DMSO: 121 mg/mL (181.21 mM); Water: 34 mg/mL (50.92 mM); Ethanol: 121 mg/mL
Identity	Confirmed by NMR/HPLC/MS.



Stability	The product is stable for three years when stored at the recommended temperature in lyophilized powder.
Applications	Vicriviroc malate can be used to study its inhibitory effects on HIV replication by targeting the CCR5 receptor.
Storage	Store at -20°C.
