



Product Information

CCR5 antagonist 1, Purity ≥98%

Cat. No.: X24-07-ZQ144

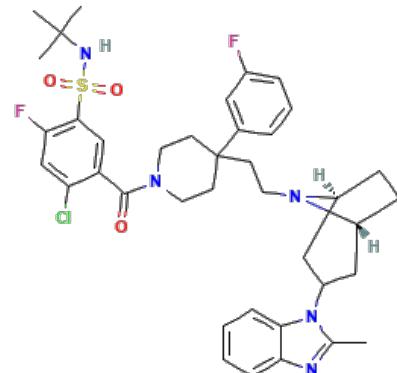
Size: 1 mg; 5 mg; 10 mg; 50 mg

CAS Number: 716354-86-8

Compound CID: 11216356

Synonym: 716354-86-8; CCR5 antagonist

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



Product Information

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| Description | CCR5 antagonist 1 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. It targets CCR5 and HIV. |
| Molecular Weight | 738.33 |
| Molecular Formula | C ₃₉ H ₄₆ ClF ₂ N ₅ O ₃ S |
| Targets | CCR5; HIV |
| IUPAC Name | <i>N</i> - <i>tert</i> -butyl-4-chloro-2-fluoro-5-[4-(3-fluorophenyl)-4-[2-[(1 <i>R</i> ,5 <i>S</i>)-3-(2-methylbenzimidazol-1-yl)-8-azabicyclo[3.2.1]octan-8-yl]ethyl]piperidine-1-carbonyl]benzenesulfonamide |
| InChI | InChI=1S/C39H46ClF2N5O3S/c1-25-43-34-10-5-6-11-35(34)47(25)30-21-28-12-13-29(22-30)46(28)19-16-39(26-8-7-9-27(41)20-26)14-17-45(18-15-39)37(48)31-23-36(33(42)24-32(31)40)51(49,50)44-38(2,3)4/h5-11,20,23-24,28-30,44H,12-19,21-22H2,1-4H3/t28-,29+,30? |
| InChI Key | ZYJBOSYROBLSKR-BWMKXQIXSA-N |
| Canonical SMILES | CC1=NC2=CC=CC=C2N1C3CC4CCC(C3)N4CCC5(CCN(CC5)C(=O)C6=CC(=C(C=C6Cl)F)S(=O)(=O)NC(C)(C)C)C7=CC(=CC=C7)F |
| Isomeric SMILES | CC1=NC2=CC=CC=C2N1C3C[C@H]4CC[C@H](C3)N4CCC5(CCN(CC5)C(=O)C6=CC(=C(C=C6Cl)F)S(=O)(=O)NC(C)(C)C)C7=CC(=CC=C7)F |
| Form | Lyophilized powder |
| Purity | ≥98% |



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| Identity | Confirmed by NMR/HPLC/MS. |
| Stability | The product is stable for three years when stored at the recommended temperature in lyophilized powder. |
| Quality Level | Research grade |
| Applications | CCR5 antagonist 1 is studied for its ability to block the CCR5 receptor, which is involved in HIV entry into cells, contributing to HIV research. |
| Storage | Store at -20°C, and keep desiccated. |
