



Product Information

CFTR inhibitor Elexacaftor, Purity $\geq 98\%$

Cat. No.: X24-07-ZQ592

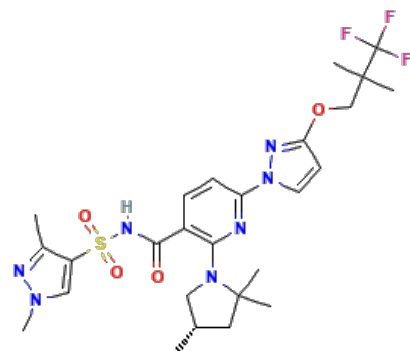
Size: 1 mg; 5 mg; 10 mg; 50 mg

CAS Number: 2216712-66-0

Compound CID: 134587348

Synonym: 2216712-66-0; CFTR inhibitor; VX-445

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



Product Information

Description	Elexacaftor, soluble in DMSO and insoluble in ethanol and water, blocks the activity of the cystic fibrosis transmembrane conductance regulator protein, which plays a crucial role in the movement of chloride ions across cell membranes.
Molecular Weight	597.65
Molecular Formula	C ₂₆ H ₃₄ F ₃ N ₇ O ₄ S
IUPAC Name	<i>N</i> -(1,3-dimethylpyrazol-4-yl)sulfonyl-6-[3-(3,3,3-trifluoro-2,2-dimethylpropoxy)pyrazol-1-yl]-2-[(4 <i>S</i>)-2,2,4-trimethylpyrrolidin-1-yl]pyridine-3-carboxamide
InChI	InChI=1S/C26H34F3N7O4S/c1-16-12-25(5,6)35(13-16)22-18(23(37)33-41(38,39)19-14-34(7)31-17(19)2)8-9-20(30-22)36-11-10-21(32-36)40-15-24(3,4)26(27,28)29/h8-11,14,16H,12-13,15H2,1-7H3,(H,33,37)/t16-m/s1
InChI Key	MVRHVFSOIWFBTE-INIZCTEOSA-N
Canonical SMILES	<chem>CC1CC(N(C1)C2=C(C=CC(=N2)N3C=CC(=N3)OCC(C)(C)C(F)(F)F)C(=O)NS(=O)(=O)C4=CN(N=C4C)C(C)C</chem>
Isomeric SMILES	<chem>C[C@H]1CC(N(C1)C2=C(C=CC(=N2)N3C=CC(=N3)OCC(C)(C)C(F)(F)F)C(=O)NS(=O)(=O)C4=CN(N=C4C)C(C)C</chem>
Form	Lyophilized powder
Purity	$\geq 98\%$
Solubility	DMSO: 99 mg/mL (165.65 mM); Water: Insoluble; Ethanol: Insoluble



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	Elexacaftor helps to study CFTR channel inhibition, important in cystic fibrosis research.
Storage	Store at -20°C, and keep desiccated.
