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Typical Product Specifications & Properties

Calcium (S)-2-(4-(((S)-2-amino-5-methyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl)methyl)amino)benza

CAS Number: : 151533-22-1

Specifications	Limits
Molecular weight	956.97
SMILES	<chem>n1c([nH]c2c(c1=O)N([C@H](CN2)CNc1ccc(cc1)C(=O)N[C@@H](CCC(=O)[O-])C(=O)[O-])C)N.[Ca+2]</chem>
InChI	VWBBRFHSPXRJQD-QNTKWALQSA-L
InChIKey	1S/C20H25N7O6.Ca/c1-27-12(9-23-16-15(27)18(31)26-20(21)25-16)8-22-11-4-2-10(3-5-11)17(30)24-13(19(32)33)6-7-14(28)29;/h2-5,12-13,22H,6-9H2,1H3,(H,24,30)(H,28,29)(H,32,33)(H4,21,23,25,26,31);/q:+2/p-2/t12-,13-;/m0./s1



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