

Typical Product Specifications & Properties

Duocarmycin B1

CAS Number: : 124325-93-5

Specifications	Limits
SMILES	<chem>N1(C[C@H](Cc2c3c(c(cc12)O)N[C@](C3=O)(C(=O)OC)C)Br)C(=O)c1[nH]c2c(c1)cc(c(c2OC)OC)OC</chem>
InChI	SUWUAMDOMCWKCL-GWQKEKGPSA-N
InChIKey	1S/C26H26BrN3O8/c1-26(25(34)38-5)23(32)18-13-8-12(27)10-30(15(13)9-16(31)20(18)29-26)24(33)14-6-11-7-17(35-2)21(36-3)22(37-4)19(11)28-14/h6-7,9,12,28-29,31H,8,10H2,1-5H3/t12-,26+/m0/s1