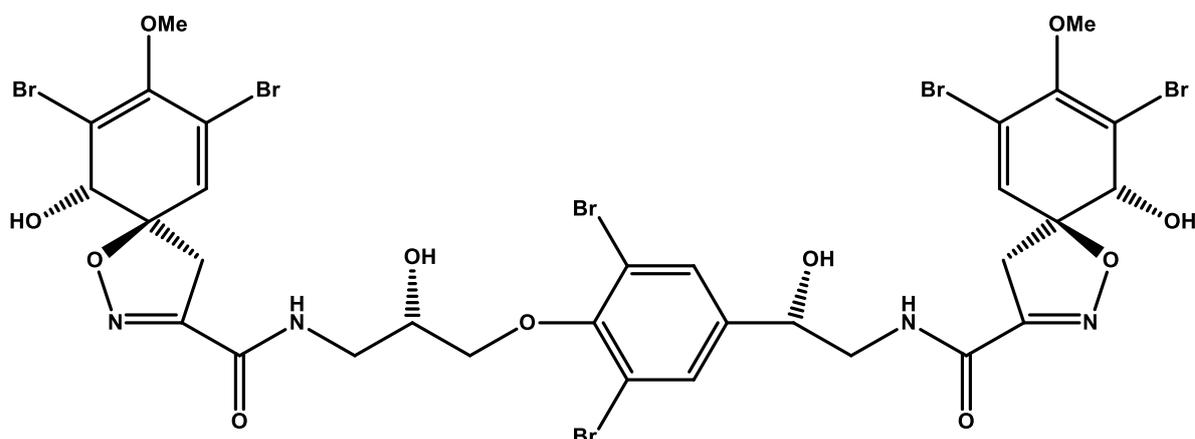


Product Data Sheet

Isofistularin-3



General description	Isofistularin-3 is a natural, marine alkaloid belonging to the group of bromotyrosine-derivatives. It is a cytotoxic isoxazoline compound and exhibits amongst others deterrent activity.
Specific biological description	<ul style="list-style-type: none"> • <i>in vitro</i> activity against HeLa cells • antiproliferative activity against Jurkat and U937 cells (MTT-Assay) • deterrent agent towards <i>B. sphinx</i> • toxic for <i>B. improvisus</i> larvae • DNMT1 inhibitor
Purity	> 99 % (HPLC)
Appearance	white to off-white solid

Product properties

Chemical name (IUPAC)	(5 <i>S</i> ,10 <i>R</i>)-7,9-dibromo- <i>N</i> -[(2 <i>R</i>)-3-[2,6-dibromo-4-[2-[[[(5 <i>S</i> ,10 <i>R</i>)-7,9-dibromo-10-hydroxy-8-methoxy-1-oxa-2-azaspiro[4.5]-deca-2,6,8-triene-3-yl]carbonyl]amino]-1-hydroxyethyl]phenoxy]-2-hydroxypropyl]-10-hydroxy-8-methoxy-1-oxa-2-azaspiro[4.5]deca-2,6,8-triene-3-carboxamide
Molecular formula	C ₃₁ H ₃₀ Br ₆ N ₄ O ₁₁
Molecular weight	1114.01 g/mol
CAS Number	87099-50-1
PubChem CID	159041
SMILES	COC1=C([C@@H])([C@]2(CC(=NO2)C(=O)NCC(COC3=C(C=C(C=C3Br)C(CNC(=O)C4=NO[C@@]5(C4)C=C(C(=C([C@@H]5

	O)Br)OC)Br)O)Br)O)C=C1Br)O)Br
Solubility	ethanol, methanol and DMSO
Source	<i>Aplysina aerophoba</i>

Product notes

Long term storage	-20 °C (protected from moisture and light)
Handling	Prepared solutions need to be stored in tightly sealed vials at -20 °C.

THIS PRODUCT IS FOR RESEARCH USE ONLY AND IS NOT INTENDED FOR DIAGNOSTIC OR THERAPEUTIC USE, NOT FOR USE IN HUMANS.

Product literature references

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- [3] B. Weiss, R. Ebel, M. Elbrächter, M. Kirchner, P. Proksch *Biochem. Syst. Ecol.* **1996**, *24*, 1.
- [4] M. S. S. Ortlepp, M. Dahlstroem, H. Weber, R. Ebel, R. Edrada, C. Thoms, P. Schupp, L. Bohlin, P. Proksch *Mar. Biotechnol.* **2007**, *9*, 776.
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- [6] C. Florean, M. Schnekenburger, J.-Y. Lee, K. R. Kim, A. Mazumder, S. Song, J.-M. Kim, C. Grandjenette, J.-G. Kim, A.-Y. Yoon, M. Dicato, K.-W. Kim, C. Christov, B.-W. Han, P. Proksch, M. Diederich *Oncotarget* **2016**, DOI: 10.18632/oncotarget.8210.