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## Typical Product Specifications & Properties

# Pectenotoxin 2

CAS Number: : 97564-91-5

Specifications	Limits
Molecular weight	859.06
SMILES	<chem>O1[C@@]([C@@H]([C@@H](CC1)C)O)([C@@H]1C[C@H]2OC([C@@H]([C@H]3O[C@]4(CC[C@H]([C@@H]([C@@]5(CC(=O)[C@H]([C@H]6C[C@@]7(C)O[C@]([C@@H]8O[C@@](C[C@H](C=C(C=C[C@H]2O1)C)C)(CC8)C)(O6)CC7)O5)C)O)O4)CCC3)C)=O)O</chem>
InChI	PTKFEDGHUVZLPL-LLUYWJARSA-N
InChIKey	1S/C47H70O14/c1-26-10-11-32-34(22-37(54-32)47(52)39(49)28(3)14-20-53-47)55-41(51)29(4)31-9-8-15-45(56-31)17-12-33(57-45)40(50)44(7)24-30(48)38(60-44)35-25-43(6)18-19-46(58-35,61-43)36-13-16-42(5,59-36)23-27(2)21-26/h10-11,21,27-29,31-40,49-50,52H,8-9



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