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## Typical Product Specifications & Properties

# Brevetoxin PbTx 1

CAS Number: : 98112-41-5

Specifications	Limits
Molecular weight	867.07
SMILES	<chem>C1[C@@H](O[C@@H]2C[C@@H]3[C@@H](O[C@@H]2[C@@H]1O)C[C@@]1(O[C@@H]2[C@@H](CCC[C@@H]1O3)O[C@@H]1[C@@H](O[C@@H]3[C@@H](CC=CC1)O[C@@H]1[C@@H](C[C@@H]3C)O[C@@]3(C[C@@H](C[C@@H]4OC(C[C@@H]4O[C@@H]3C1)=O)C)C)CC=C2)C)C</chem>
InChI	MGVIMUPHKPHT KF-PMAMELDRSA-N
InChIKey	1S/C49H70O13/c1-26-17-36-39(22-45(52)58-36)57-44-21-38-40(48(44,4)23-26)18-28(3)46-35(55-38)11-7-6-10-31-32(59-46)12-8-131)13-9-15-43-49(5,61-34)24-42-37(56-43)20-41-47(60-42)30(51)41)16-27(2)25-50/h6-8,14,25-26,28-44,46-47,51H,



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