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## Typical Product Specifications & Properties

# CAERULEIN

CAS Number: : 17650-98-5

Specifications	Limits
Molecular weight	1,352.42
SMILES	<chem>C1CC(N[C@@H]1C(N[C@H](C(=O)N[C@@H](CC(O)=O)C(=O)(C(N[C@@H]([C@@H](C)O)C(=O)NCC(=O)N[C@H](C(N[C@@H](CCSC)C(N[C@@H](CC(O)=O)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)=O)=O)Cc1c[nH]c2ccccc12)=O)Cc1c(=O)O)CCC(N)=O)=O</chem>
InChI	YRALAIOMGQZ KOW-HYAOXDFASA-N
InChIKey	1S/C58H73N13O21S2/c1-29(72)49(71-57(87)40(23-31-12-14-33(94(89,90)91)68-56(86)43(26-48(78)79)69-52(82)37(16-18-44(59)51(81)36-17-19-45(74)63-36)58(88)62-28-46(75)64-41(24-32-27-634(32)35)54(84)66-38(20-21-93-2)53(83)70
Chemical Structure	 45192_45192_caerulein.png chemical structure



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