

Product Data Sheet

Product Name: Emestrin
Cat. No.: GC46137

Chemical Properties

Cas. No. 97816-62-1

SMILES OC(C=CC([C@@H]([C@]1(SS2)N(C)C([C@]2([C@H](O)C3=COC=CC(OC4=O)[C@]35[H])N5C1=O)=O)O)=C6)=C6OC7=CC4=CC=C7OC

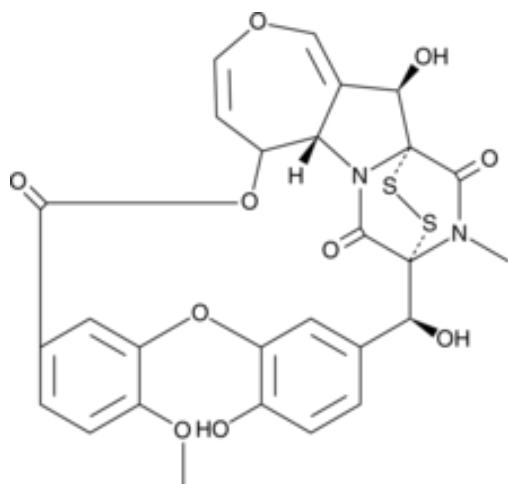
Formula C₂₇H₂₂N₂O₁₀S₂ M.Wt 598.6

Solubility DMF: soluble, DMSO: Storage Store at -20°C
soluble, Ethanol: soluble, Methanol: soluble

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

Emestrin is a mycotoxin originally isolated from *E. striata* that has antimicrobial, immunomodulatory, and cytotoxic activities.^{1,2,3,4,5} It is active against the fungi *C. albicans* and *C. neoformans*, as well as the bacteria *E. coli*, *S. aureus*, and methicillin-resistant *S. aureus* (MRSA; IC₅₀s = 3.94, 0.6, 2.21, 4.55, and 2.21 µg/ml, respectively).² Emestrin is a chemokine (C-C motif) receptor 2 (CCR2)

Caution: Product has not been fully validated for medical applications. For research use only.

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antagonist (IC₅₀ = 5.4 μ M in a radioligand binding assay using isolated human monocytes).³ Emestrin (0.1 μ g/ml) induces apoptosis in HL-60 cells.⁴ It induces heart, thymus, and liver tissue necrosis in mice when administered at doses ranging from 18 to 30 mg/kg.⁵

[1. Seya, H., Nakajima, S., Kawai, K.-i., et al. Structure and absolute configuration of emestrin, a new macrocyclic epidithiodioxopiperazine from *Emericella striata*. J. Chem. Soc. Chem. Commun. 10, 657-658 (1985).]2. Herath, H.M.T.B., Jacob, M., Wilson, A.D., et al. New secondary metabolites from bioactive extracts of the fungus *Armillaria tabescens*. Nat. Prod. Res. 27(17), 1562-1568 (2013).]3. Herath, K.B., Jayasuriya, H., Ondeyka, J.G., et al. Isolation and structures of novel fungal metabolites as chemokine receptor (CCR2) antagonists. J. Antibiot. (Tokyo) 58(11), 686-694 (2005).]4. Ueno, Y., Umemori, K., Niimi, E.-c., et al. Induction of apoptosis by T-2 toxin and other natural toxins in HL-60 human promyelotic leukemia cells. Nat. Toxins 3(3), 129-137 (1995).]5. Terao, K., Ito, E., Kawai, K.-i., et al. Experimental acute poisoning in mice induced by emestrin, a new mycotoxin isolated from *Emericella* species. Mycopathologia 112(2), 71-79 (1990).

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