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Structural Analysis of ATHOD The Fatty Amino Acid and ATHOD-containing Peptides Burkholdines and Occidiofungins

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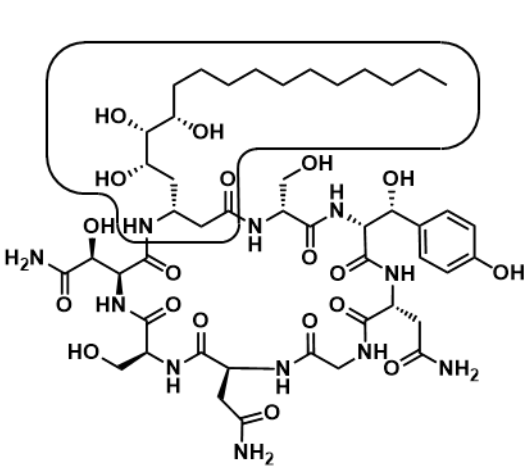
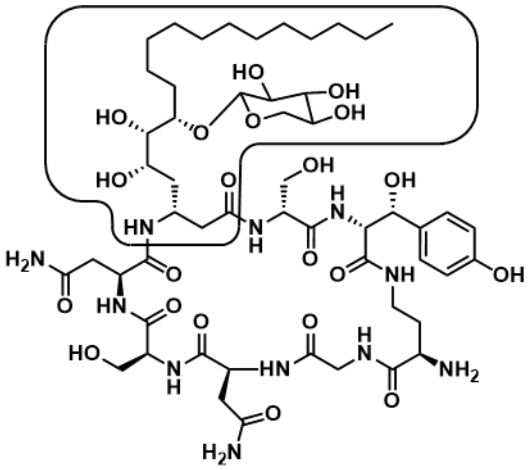
Burkholdine-1097 (Bk-1097) is a cyclic lipopeptide isolated in 2010 and has potent antifungal activities. However, total synthesis of Bk-1097 has not been achieved and its mechanism of action have not been revealed. Although we have conducted synthetic study of Bk analogs, we have never synthesized 3-amino-5,6,7-trihydroxy octadecanoic acid (ATHOD) moiety. Therefore, we report the synthesis of the protected ATHOD derivatives and elucidation of the absolute configuration.

we carried out ^{1}H-NMR analysis of 8 diastereo isomers of the ATHOD derivatives prepared by us and reported compounds based on the Kishi's NMR database method. The stereochemistry of 1,3-amino alcohol moiety was determined from the Marfey's analysis and the comparison of known compounds. The absolute configuration of the ATHOD moiety of Bk-1097 was determined to be (3*R*,5*S*,6*R*,7*S*) although those of isolated Bk-1097 was reported as (3*R*,5*R*,6*S*,7*S*).

Furthermore, we revised the assignment of the NMR data of Bks family by further structural analysis and determined that the absolute configuration of the ATHOD moiety of occidiofungin A that has similar chemical structure and antifungal activity[1].



Bk-1097



Occidiofungin A

1) Kadowaki, T.; Kainuma, R.; Kato, S.; Konno, H. *J. Nat. Prod.* **2022**, 2052-2061.