Structural Reassignment of the Antibiotic A53868 Reveals a Tripeptide with an Unusual Amino Dehydrophosphonic Acid Monomethylester.

John T. Whitteck and Wilfred A. van der Donk

The phosphonate antibiotic A53868 was isolated in 1984 and originally assigned as structure **1**, but was later changed to structure **2**. After our lab synthesized **2**, it was found that the structure was spectroscopically inconsistent with the isolated material. A combination of ¹H, ¹³C, ³¹P NMR and HRMS were used with non-labeled, ¹⁵N- and ¹³C¹⁵N- labeled A53868 to identify the actual structure as **3**. The first total synthesis of **3** showed the structure to be spectroscopically identical to isolated A53868, which reveals unique structural characteristics and raises questions as to its biosynthesis and mode of action.