

Crystal Structures Puzzle of the DSDH Gramicidin Channel

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The naturally occurring antibiotic gramicidin forms transmembrane channels specific for monovalent cations. In a solution several polymorphic gramicidin forms have been observed. All uncomplexed gramicidin crystal structures are reported to be left-handed antiparallel double-stranded double-helix (DSDH) dimers with 5.6 residues per turn. The same form was also observed by NMR in organic solvents. In contrast there are conflicting results concerning the crystal structures of complexed gramicidin. Despite the same space group and cell dimensions that agree to within 0.1%, two entirely different three-dimensional structures have been reported. Both structures contain DSDH dimers but they differ in h.b. patterns and the overall hand of the helices. The **right-handed** form agrees with NMR data in organic solvents, while no NMR data supporting the **left-handed** structure exists. Furthermore, the crystallographic, stereochemical, and chemical anomalies of the latter form suggest that the structure determination could be erroneous. Unfortunately, the reluctance of the authors to release their intensity data makes it impossible to unequivocally set to rest the question.

Therefore, we have made a thorough analysis of the two complexed gramicidin structures in question, including energy calculations and refinement of the LH form basing on RH diffraction data. (Research Project 3 T09A 047 26 from KBN).

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