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Antimicrobial peptide protegrin-3 adopt an antiparallel dimer in the presence of DPC micelles: A high-resolution NMR study

Usachev K., Efimov S., Kolosova O., Klochkova E., Aganov A., Klochkov V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 Springer Science+Business Media Dordrecht. A tendency to dimerize in the presence of lipids was found for the protegrin. The dimer formation by the protegrin-1 (PG-1) is the first step for further oligomeric membrane pore formation. Generally there are two distinct model of PG-1 dimerization in either a parallel or antiparallel β -sheet. But despite the wealth of data available today, protegrin dimer structure and pore formation is still not completely understood. In order to investigate a more detailed dimerization process of PG-1 and if it will be the same for another type of protegrins, in this work we used a high-resolution NMR spectroscopy for structure determination of protegrin-3 (RGGGL-CYCRR-RFCVC-VGR) in the presence of perdeuterated DPC micelles and demonstrate that PG-3 forms an antiparallel NCCN dimer with a possible association of these dimers. This structural study complements previously published solution, solid state and computational studies of PG-1 in various environments and validate the potential of mean force simulations of PG-1 dimers and association of dimers to form octameric or decameric β -barrels.

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Keywords

Antimicrobial peptide, Dimer, DPC micelle, NMR, Protegrin, Structure