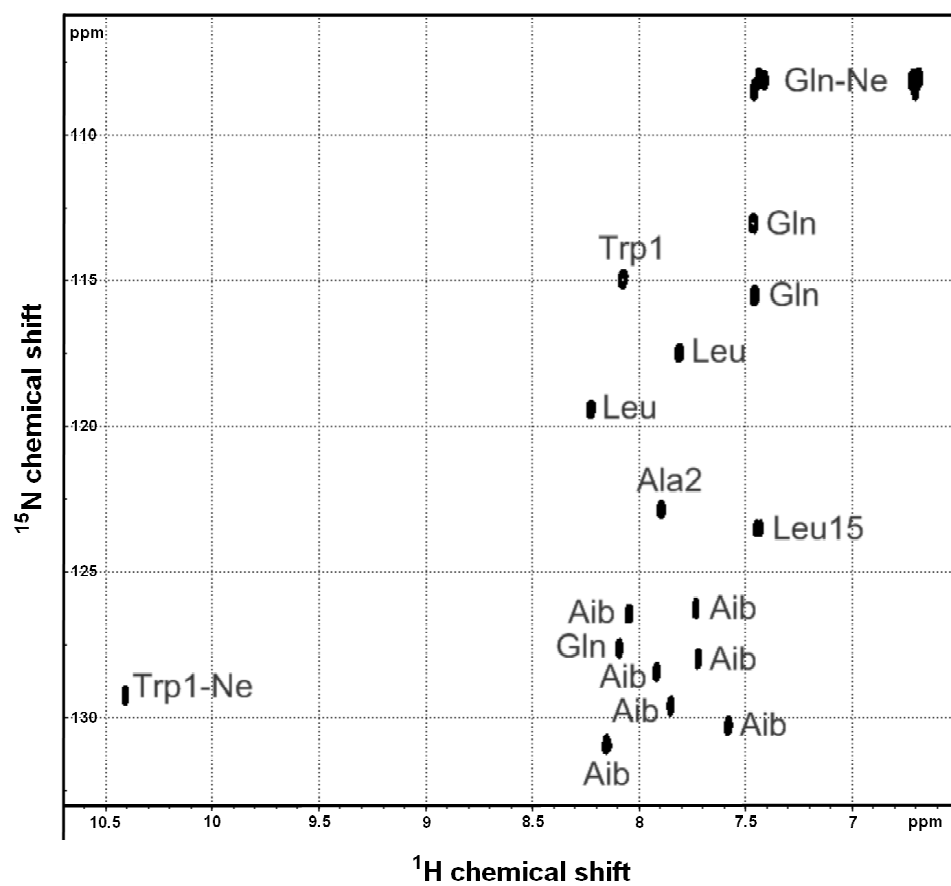


Supplementary Material

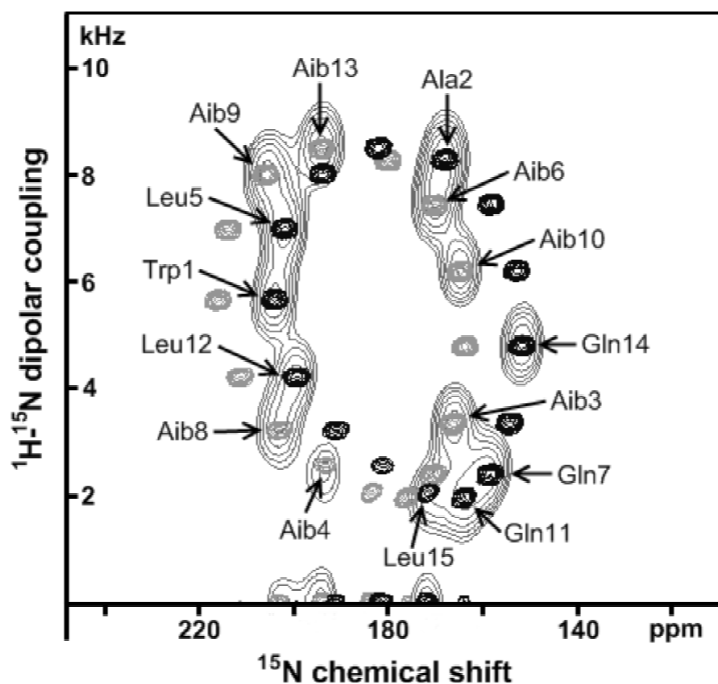
**Structure and alignment of the membrane-associated peptaibols
ampullosporin A and alamethicin by oriented ^{15}N and ^{31}P solid-state
NMR spectroscopy**

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Bechinger**

SUPPLEMENTARY INFORMATION



Supplementary Figure S1. HSQC spectrum of uniformly ^{15}N labeled AmpA in CD_3OH .



Supplementary Figure S2: The light grey spectrum exhibiting broadened line shapes shows the simulation of the PISEMA spectrum of an ideal α -helix composed of the AmpA sequence at an alignment that best represents the experimental spectrum observed in di-C10:0-PC (cf. Fig. 4C). The tensor elements are ($\delta_{\text{iso}}=129.5$ ppm, $\delta_{\text{aniso}}=105$ ppm, $\eta=0.2$) for the Aib residues and ($\delta_{\text{iso}}=117.5$ ppm, $\delta_{\text{aniso}}=105$ ppm, $\eta=0.2$) for all other amino acid residues. The simulated line-width are 300 Hz in the ^{15}N chemical shift- and 1 kHz in the dipolar coupling dimension. In order to illustrate how the simulated pattern arises from two ('incomplete') helical wheels that are shifted by 12 ppm from each other the corresponding PISA wheels (encompassing a complete set of 15 pitch angles) are shown as grey dots for ($\delta_{\text{iso}}=117.5$ ppm, $\delta_{\text{aniso}}=105$ ppm, $\eta=0.2$) and as black dots for ($\delta_{\text{iso}}=129.5$ ppm, $\delta_{\text{aniso}}=105$ ppm, $\eta=0.2$). The assignments point to those residues that compose the simulated AmpA helical spectrum (Fig. 4C).

Ampullosporin A Production

Table S1: Ampullosporin A production in liquid and solid media

Medium	Duration of incubation	ampullosporin A ($\mu\text{g} / 100 \text{ ml}$)
Liquid medium 1	6 Weeks	395,6
Liquid medium 2	6 Weeks	2,31
Liquid medium 3	6 Weeks	1018,1
Liquid medium 4	6 Weeks	142,2
Liquid medium 5	6 Weeks	516,0
Liquid medium 6	6 Weeks	22,1
Liquid medium 7	3 Weeks	1206,6
Liquid medium 8	3 Weeks	908,5
Liquid medium 9	3 Weeks	615,9
Liquid medium 10	3 Weeks	321,4
Solid medium 1	6 Weeks	264,1
Solid medium 2	6 Weeks	43,5
Solid medium 3	6 Weeks	39,4
Solid medium 4	6 Weeks	6,7
Solid medium 5	6 Weeks	66,8
Solid medium 6	6 Weeks	0,8
Solid medium 7	3 Weeks	536,3
Solid medium 8	3 Weeks	366,9
Solid medium 9	3 Weeks	300,9
Solid medium 10	3 Weeks	329,1

Media

Malt Medium (MA)	40 g Malt extract, 4 g Yeast extract
Medium 1	10 g Glucose, 3,5 g $(\text{NH}_4)_2\text{SO}_4$, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$
Medium 2	Medium 1 + 5,1 g CaCO_3
Medium 3	10 g Maltose, 3,5 g $(\text{NH}_4)_2\text{SO}_4$, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$
Medium 4	Medium 3 + 5,1 g CaCO_3
Medium 5	20 g Maltose, 3,5 g $(\text{NH}_4)_2\text{SO}_4$, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$
Medium 6	Medium 5 + 5,1 g CaCO_3
Medium 7	5 g Maltose, 2 g Caseine Pepton, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$, pH 5,8 - 6,2
Medium 7*	5 g Maltose, 2 g Celtone- ^{15}N , 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$, pH 5,8 - 6,2
Medium 8	10 g Maltose, 2 g Caseine Pepton, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$, pH 5,8 - 6,2
Medium 9	5 g Glukose, 2 g Caseine Pepton, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$, pH 5,8 - 6,2
Medium 10	10 g Glukose, 2 g Caseine Pepton, 2,0 g KH_2PO_4 , 0,5 g $\text{MgSO}_4 \times 7 \text{ H}_2\text{O}$, 0,008 g $\text{ZnSO}_4 \times 7 \text{ H}_2\text{O}$, pH 5,8 - 6,2

MK Agar
39 g / l, pH 5,6)

1:1 Malt agar / Potatoe-Glucose-Agar (Fertigagar Merck,