Models for gramicidin channels

To the Editor:

In several recent papers, NMR results for gramicidin A have been compared with predictions based on various models for a right-handed channel. In particular, ²H quadrupolar splittings (Hing et al., 1990a,b; Prosser et al., 1991) or ¹⁵N chemical shifts (Chiu et al., 1991) from solid-state NMR spectra of labeled gramicidin A in oriented phospholipid multilayers have been compared to the values that would be predicted for a righthanded model derived from model-building considerations (Koeppe and Kimura, 1984) and to values predicted by a preliminary model based on 2-dimensional ¹H NMR data for gramicidin in SDS (Arseniev et al., 1985). These latter authors have, however, published an updated model that was derived from their NMR data for gramicidin in SDS (Arseniev et al., 1986). This updated model was based upon additional experimental results and corrected many of the inconsistencies in the original Arseniev model. It would therefore be appropriate to use the 1986 Arseniev model in preference to the 1985 model for comparisons with experimental data. Stereo pictures of the updated Arseniev model for the right-handed gramicidin A channel and its mirror image have recently been published (Koeppe et al., 1992).

Received for publication 4 November 1991.

REFERENCES

Arseniev, A. S., I. L. Barsukov, V. F. Bystrov, A. L. Lomize, and Y. A. Ovchinnikov. 1985. Proton NMR study of gramicidin A transmembrane ion channel. Head-to-head right-handed, single-stranded helixes. FEBS (Fed. Eur. Biochem. Soc.) Lett. 186:168–174.

- Arseniev, A. S., A. L. Lomize, I. L. Barsukov, and V. F. Bystrov. 1986. Gramicidin A transmembrane ion-channel. Three-dimensional structure reconstruction based on NMR spectroscopy and energy refinement. *Biol. Membr.* 3:1077-1104. (In Russian).
- Chiu, S. W., L. K. Nicholson, M. T. Brenneman, S. Subramaniam, Q. Teng, J. A. McCammon, T. A. Cross, and E. Jakobsson. 1991.
 Molecular dynamics computations and solid state nuclear magnetic resonance of the gramicidin cation channel. *Biophys. J.* 60:974–978.
- Hing, A. W., S. P. Adams, D. F. Silbert, and R. E. Norberg. 1990a. Deuterium NMR of Val¹ . . . (2-²H)Ala³ . . . gramicidin A in oriented DMPC bilayers. *Biochemistry*. 19:4144–4156.
- Hing, A. W., S. P. Adams, D. F. Silbert, and R. E. Norberg. 1990b. Deuterium NMR of ²HCO-Val¹...gramicidin A and ²HCO-Val¹-D-Leu²...gramicidin A in oriented DMPC bilayers. *Biochemistry*. 29:4156–4166.
- Koeppe, R. E., II, and M. Kimura. 1984. Computer building of β-helical polypeptide models. *Biopolymers*. 23:23–38.
- Koeppe, R. E., II, L. L. Providence, D. V. Greathouse, F. Heitz, Y. Trudelle, N. Purdie, and O. S. Andersen. 1992. On the helix sense of gramicidin A single channels. *Proteins*. 12:49–62.
- Prosser, R. S., J. H. Davis, F. W. Dahlquist, and M. A. Lindorfer. 1991. Deuterium nuclear magnetic resonance of the gramicidin A backbone in a phospholipid bilayer. *Biochemistry*. 30:4687–4696.

Roger E. Koeppe II,* M. Jeff Taylor,* Olaf S. Andersen*
*Department of Chemistry and Biochemistry
University of Arkansas

Fayetteville, Arkansas 72701; and †Department of Physiology and Biophysics Cornell University Medical College

New York, New York 10021 USA