



JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1998, 120(17), 4236-4237, DOI:[10.1021/ja973704q](https://doi.org/10.1021/ja973704q)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

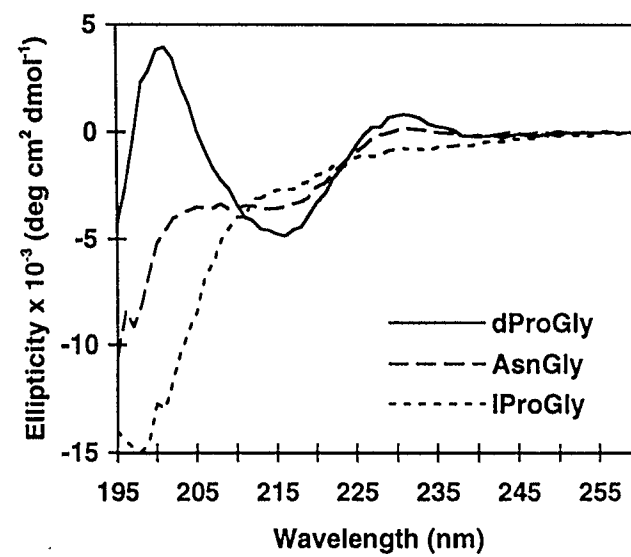
SUPPLEMENTARY FIGURE CAPTIONS

Supplementary Figure 1. Circular dichroism data for 0.10 mM ^DPG (solid), 0.15 mM NG (dashed) and 0.10 mM ^LPG (dotted) in 100 mM aqueous sodium acetate buffer, pH 3.8, 25°C. Data obtained on an Aviv 62 ADS spectrometer.

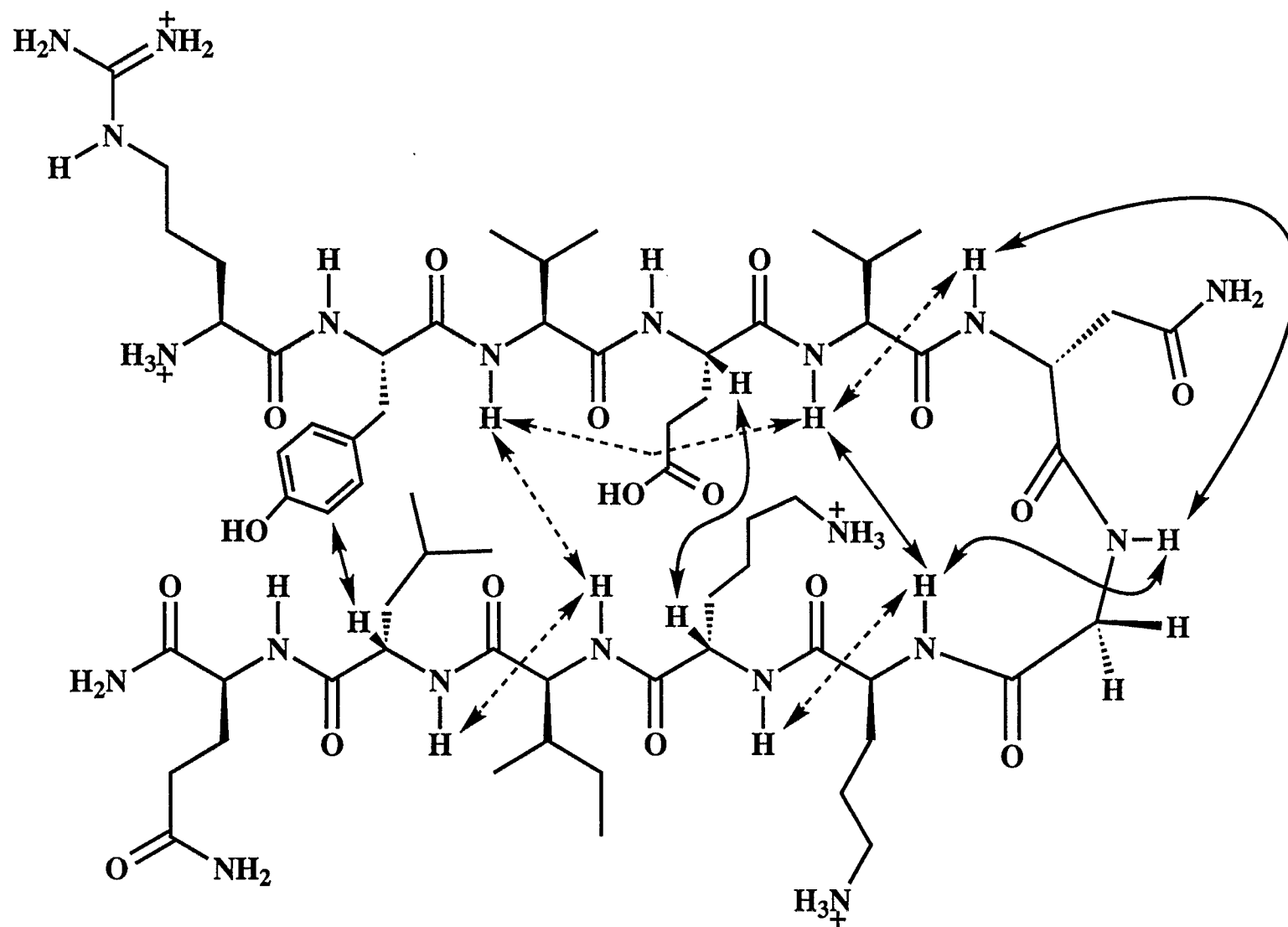
Unlike the CD data in this Figure, the ROESY data summarized in Figure 1 in the text were obtained at 4°C. ROESY data obtained for ^DPG at 25°C showed numerous cross-strand NOEs consistent with β -hairpin folding, but there were fewer cross-strand NOEs at 25°C than at 4°C. NOEs not observed at 25°C included the NH--NH NOE between Val-3 and Ile-10, and several of the side chain-side chain NOEs among Tyr-2, Lys-9 and Leu-11. The non-hairpin NOE mentioned in the text was also not observed at 25°C, but a new non-hairpin NOE was observed at this higher temperature, between Tyr-2 δ -CH and Ile-10 γ -CH₂.

Supplementary Figure 2. Long-range NOEs observed in ROESY analysis for 4.6 mM NG in 100 mM aqueous sodium deuterioacetate buffer, pH 3.8 (uncorrected), 4°C. (A) NOEs involving NH and/or H α resonances (H α --H α NOEs were observed in D₂O, and the remaining NOEs in 9:1 H₂O:D₂O). Dotted lines indicate weak NOEs. (B) NOEs involving side chains (obtained in 9:1 H₂O:D₂O). Resonance assignments were obtained from a combination of COSY and TOCSY data, and sequential NOEs from ROESY data.

Supplementary Figure 1.



Supplementary Figure 2(A).



Supplementary Figure 2(B).

