An electronic effect on protein structure

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**NOESY 1D spectroscopy**

All NOESY 1D experiments were performed on a Varian UNITY-500 spectrometer. Representative spectra of N-formyl-L-proline methyl ester are shown on p 3 and 4. Irradiation of the α-proton resonances at 4.5 ppm produced a strong NOE at 8.08 ppm, which was assigned as the cis formyl proton resonance. Irradiation of the δ-protons at 3.5 ppm produced a strong NOE at 8.14 ppm, which was assigned as the trans formyl proton resonance. Key parameters: Mix = 4.0 s, d1 = 10.6 s, tpwr = 63.

**FTIR spectroscopy**

FTIR spectra were recorded on NaCl plates with a Mattson Infinity FTIR spectrometer and verified on a Mattson Polaris spectrometer. Experiments were performed at 25 °C. All samples were prepared as neat oils.
Compound 1
$^1$H NMR 500 MHz in D$_2$O

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Compound 1
Irradiated at the alpha proton
NOESY 1D in D$_2$O
Varian UNITY-500
Compound 1
Irradiated at the delta protons
NOESY 1D in D$_2$O
Varian UNITY-500
Compound 1
250 MHz in CDCl₃

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Compound 1
500 MHz in dioxane-D$_8$

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Compound 1
75 MHz in CDCl₃

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Compound 2
500 MHz in CDCl₃

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Compound 2
500 MHz in dioxane-D$_8$

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Compound 2
75 MHz in CDCl₃

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Compound 3
500 MHz in CDCl₃

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Compound 3
500 MHz in dioxane-D8

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Compound 3
250 MHz in D$_2$O

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Compound 3
75 MHz in CDCl₃

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Infrared Spectrum of \( N \)-Formylproline Methyl Ester

\begin{align*}
\text{Transmittance (\%)} & \quad 90 \\
\text{Wavenumber} & \quad 4000 \quad 3500 \quad 3000 \quad 2500 \quad 2000 \quad 1500 \quad 1000
\end{align*}

1742.8

1672.1

\[ \text{N} \quad \text{H} \quad \text{O} \quad \text{O} \quad \text{O} \quad \text{H} \quad \text{O} \]

Infrared Spectrum of \( N \)-Formylproline Methyl Ester

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Infrared Spectrum of *N*-Acetylproline Methyl Ester

Transmittance (%)

Wavenumber

4000 3500 3000 2500 2000 1500 1000

70 75 80 85 90

1742.0

1642.3

H3C

CO

N

C

O