Supplementary Material for PCCP

STUDY OF CONFORMATIONAL PROPERTIES OF A BIOLOGICALLY ACTIVE PEPTIDE OF FIBRONECTIN BY CIRCULAR DICHROISM, NMR AND MOLECULAR DYNAMICS SIMULATION

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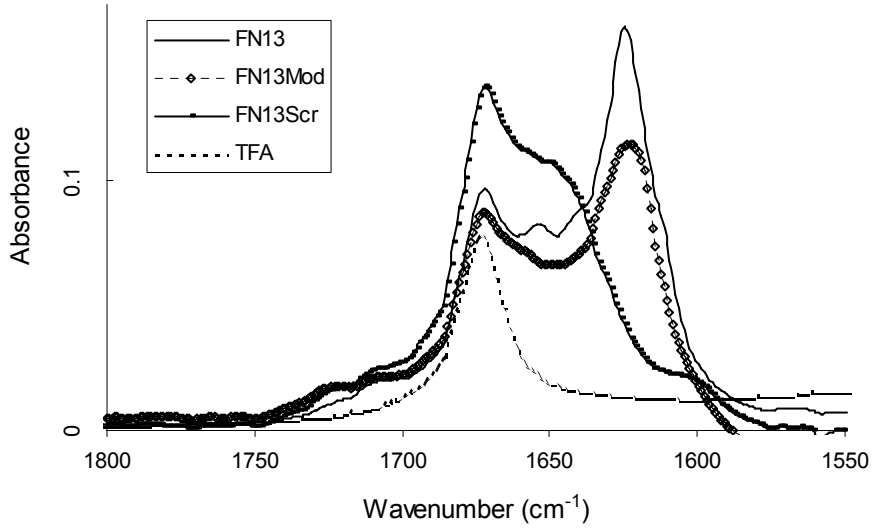
IR spectroscopy. FTIR measurements were recorded with a JASCO FVS-4000 spectrometer. Peptides solutions were prepared in D_2O at a concentration of about 1.4 % (w/w). After an equilibration time of at least 24h for H/D exchange, the IR experiments were run by placing a small amount of solution between two BaF2 windows separated with a 25 μm Teflon spacer.
The peptide samples were used without removing the residual trifluoracetic acid (TFA) whose absorption around 1673 cm^{-1} may interfere with the amide band [*J.Hilario, J. Kubelka, T. Keiderling, J. Am. Chem. Soc., **2003**, 125, 7562*].

The figure presents the absorption spectra of the three peptides: FN13, FN13Mod, FN13Scr from which the D_2O absorption has been subtracted. The TFA spectrum (a.u.) is also presented for comparison.



Despite the presence in the samples of a residual amount of TFA, yet these preliminary results suggest different behaviour between the scrambled and the other peptides: the native (FN13) and the modified peptides (FN13Mod) present an absorption band at 1625 cm^{-1} which is not present for the scrambled (FN13Scr).