

Supporting Information

An amyloid-like fibril-forming supramolecular cross- β -structure of a model peptide: a crystallographic insight

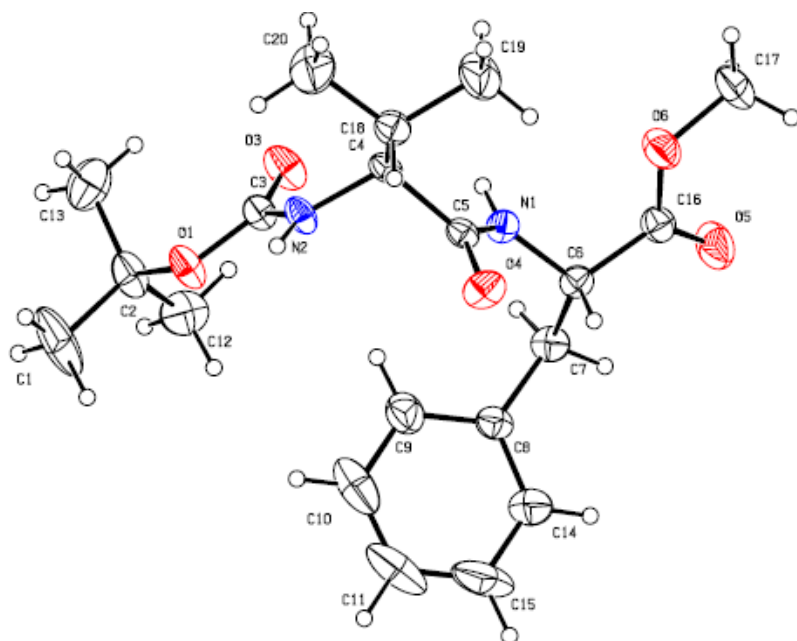
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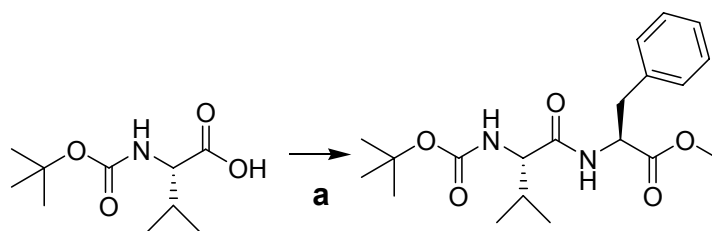
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ESI Figure S1: The ORTEP diagram of peptide **1** showing the atomic numbering scheme.

Ellipsoids are drawn at the 30% probability level.



Scheme 1: Schematic presentation of synthesis of peptide **1**. Reagents and conditions: a) DCM, H-Phe-OMe, DCC, HOBT, 0°C.

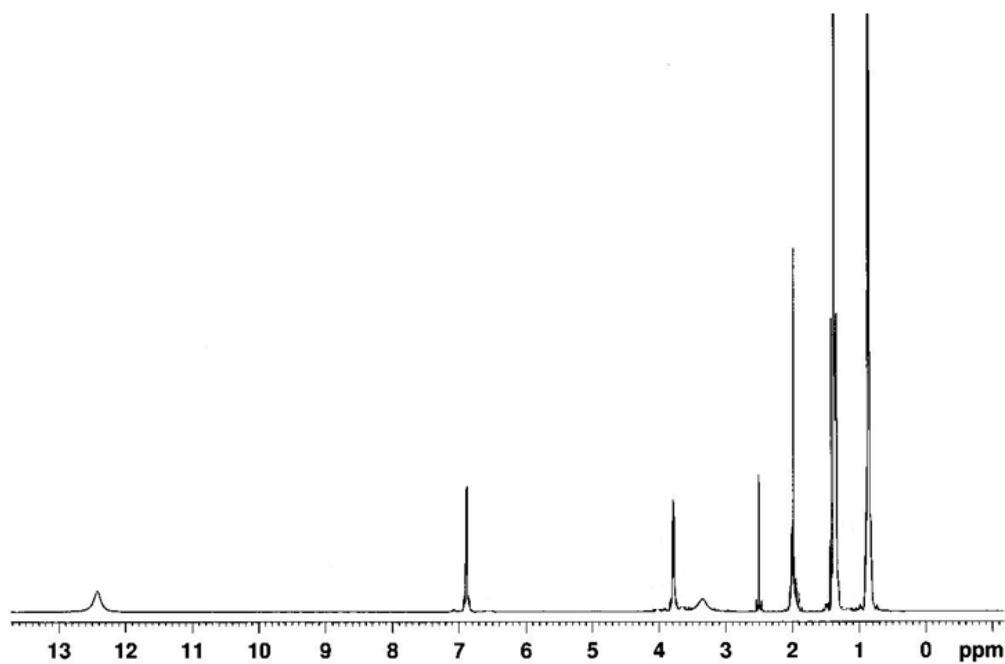
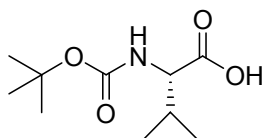


Figure S2: ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectra of Boc-Val(1)-OH 2.

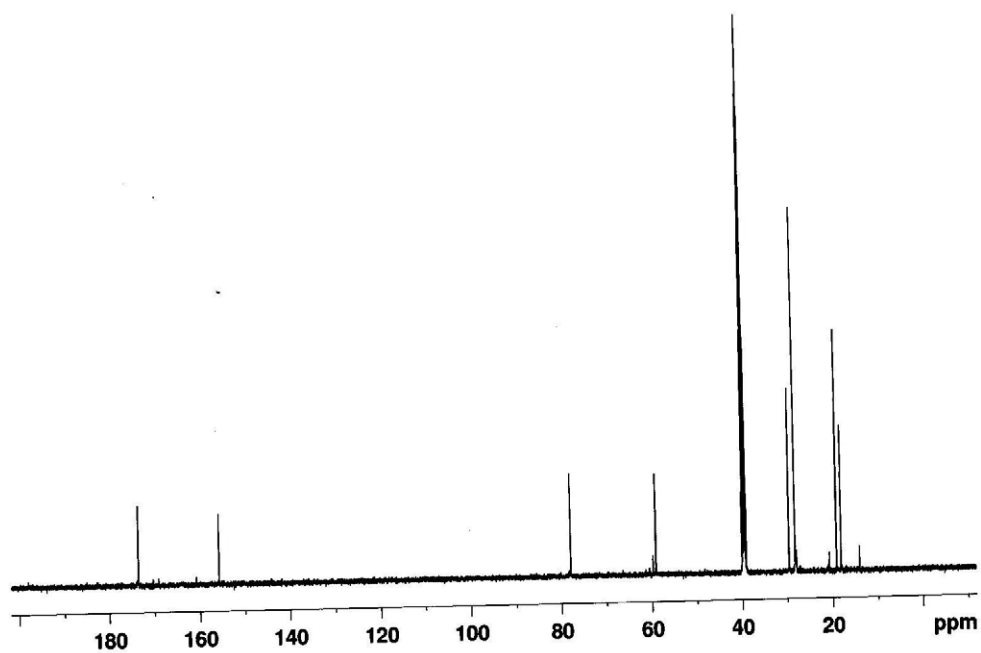


Figure S3: ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) spectra of Boc-Val(1)-OH 2.

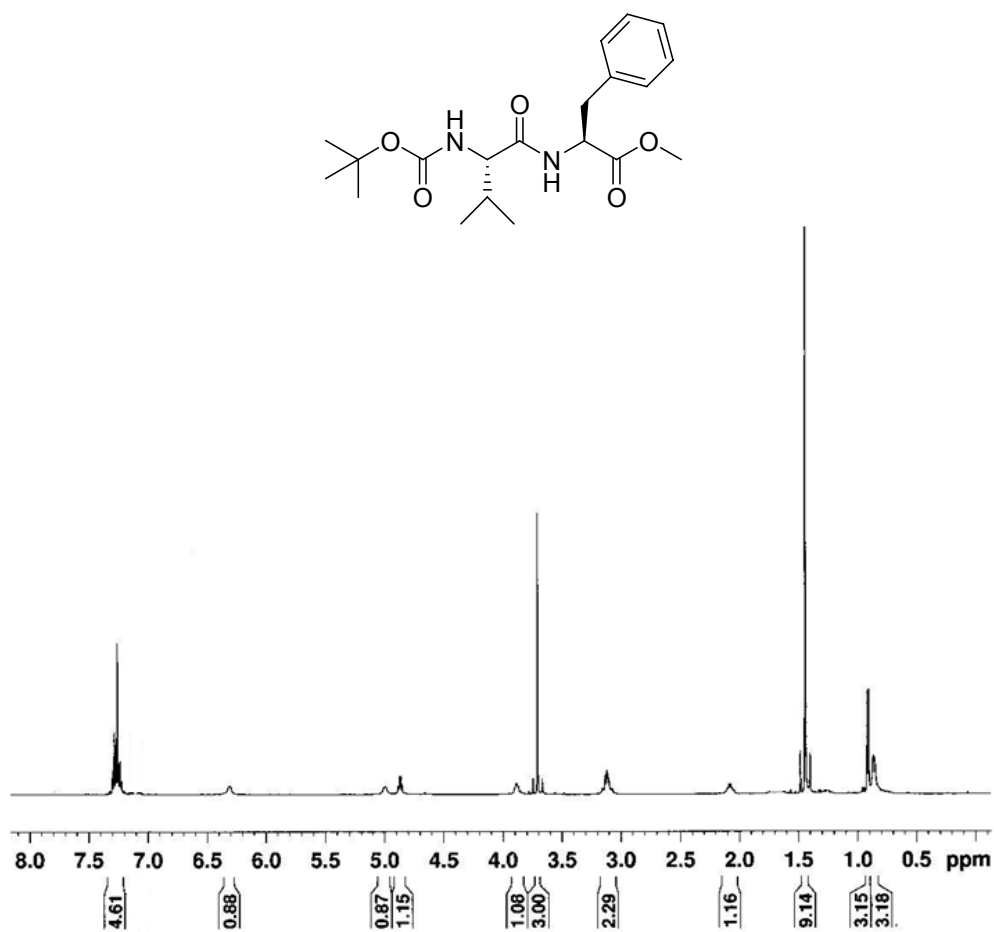


Figure S4: ¹H NMR (500 MHz, CDCl₃) spectra of Boc-Val(1)-Phe(2)-OMe 1.

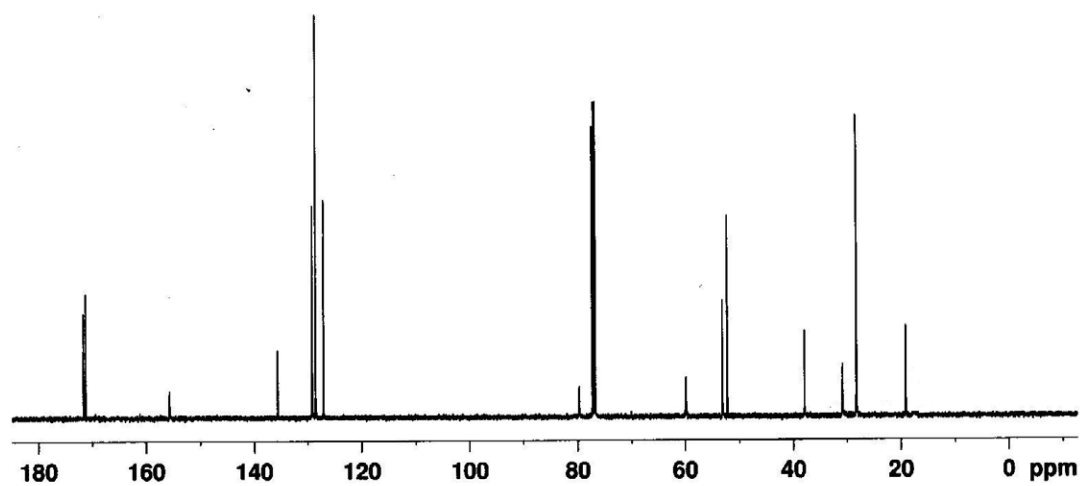


Figure S5: ¹³C NMR (125 MHz, CDCl₃) spectra of Boc-Val(1)-Phe(2)-OMe 1.

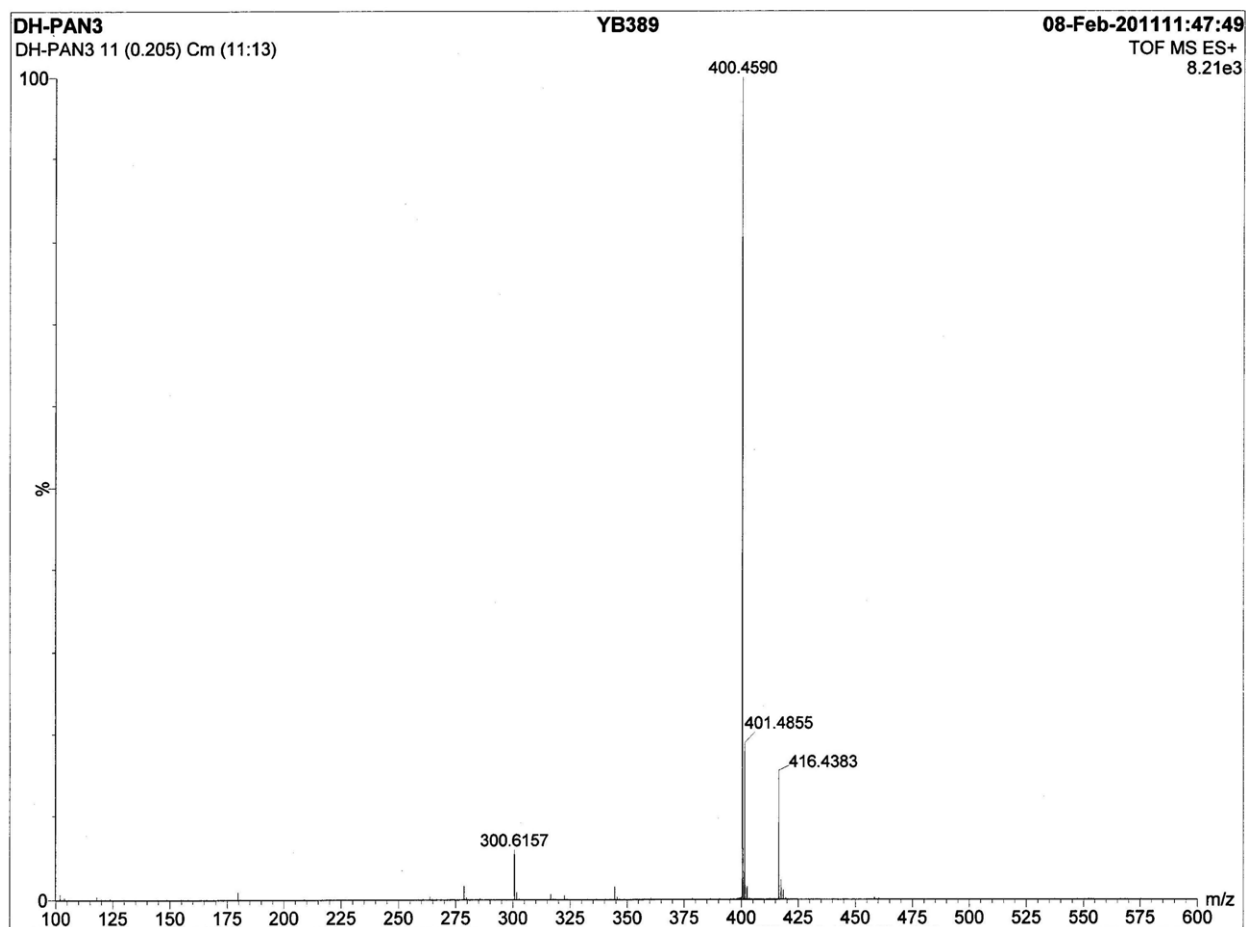


Figure S6: Mass spectra of Boc-Val-Phe-OMe 1.

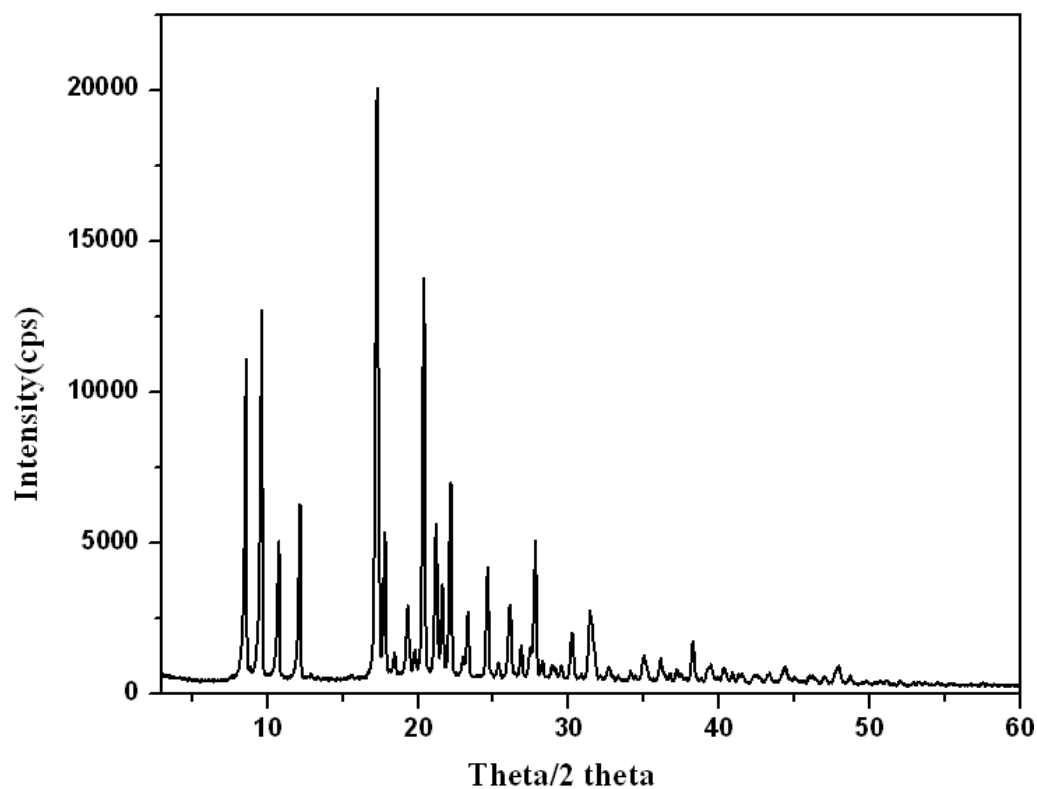


Figure S7: X-ray diffraction data obtained from Boc-Val-Phe-OMe 1 fibrils.

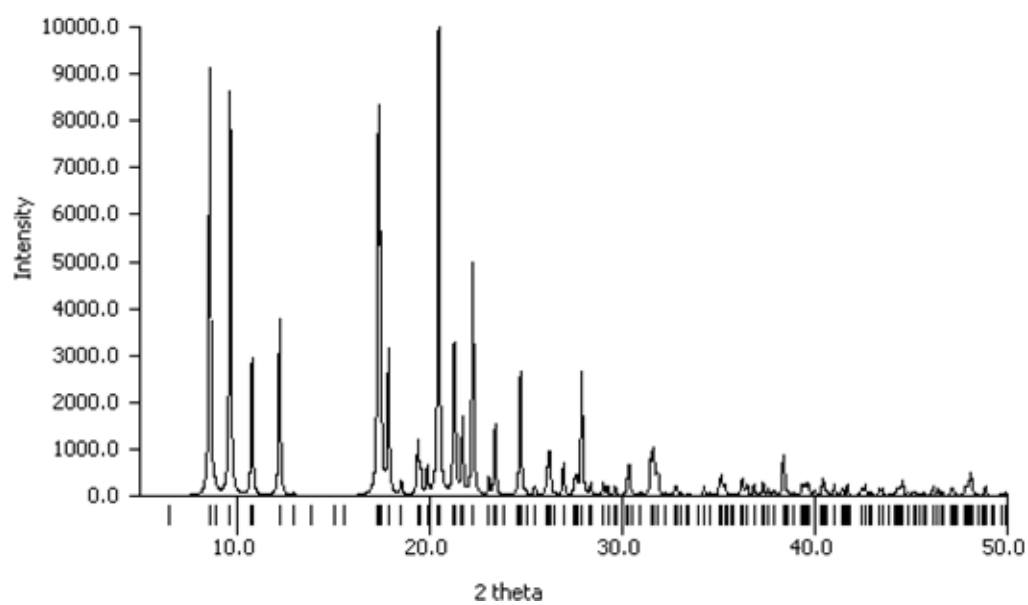


Figure S8: Powder pattern from X-ray crystallography of Boc-Val-Phe-OMe 1.