

Supporting information

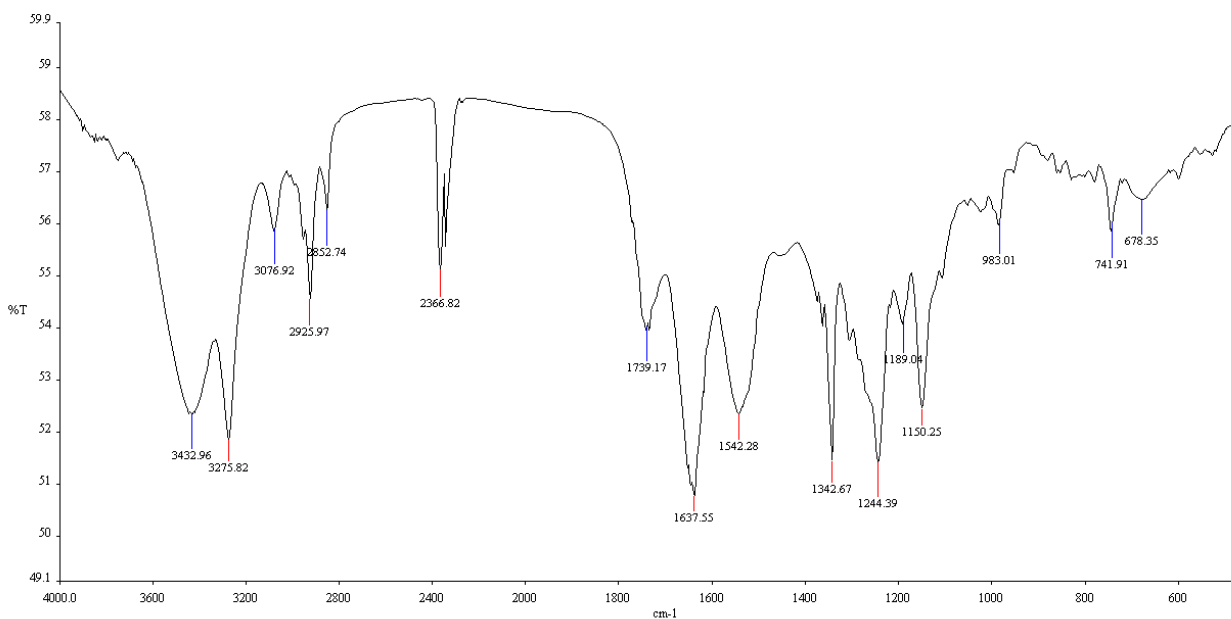
Self-assembly and nonlinear optical property of a synthetic dipeptide †

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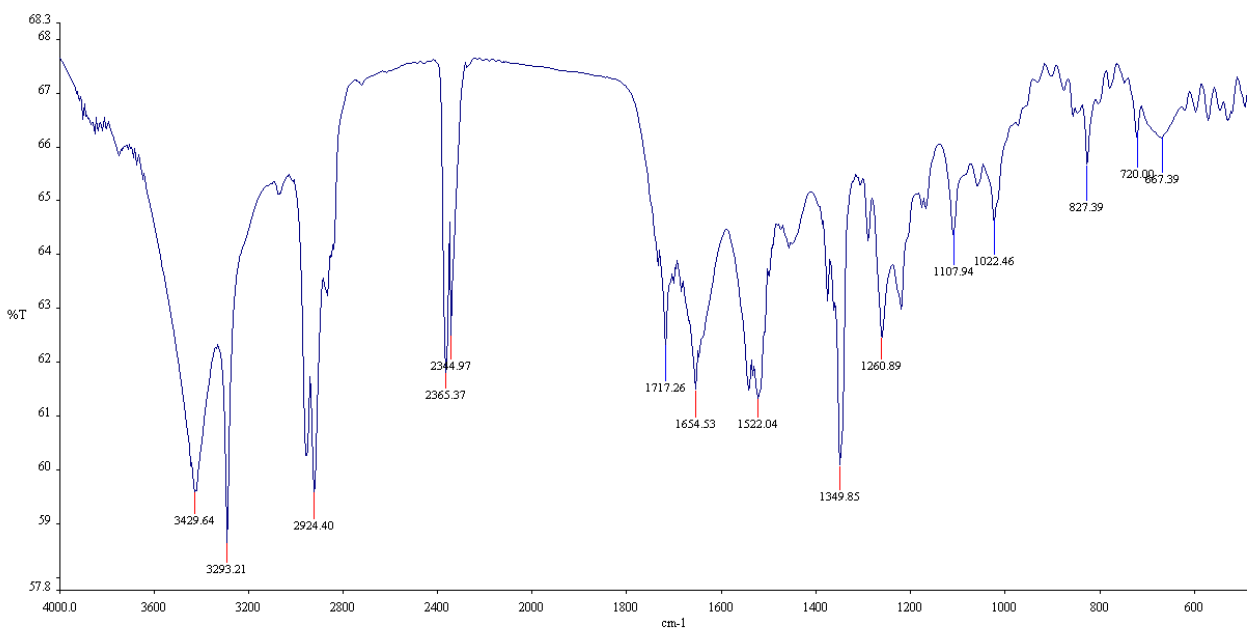
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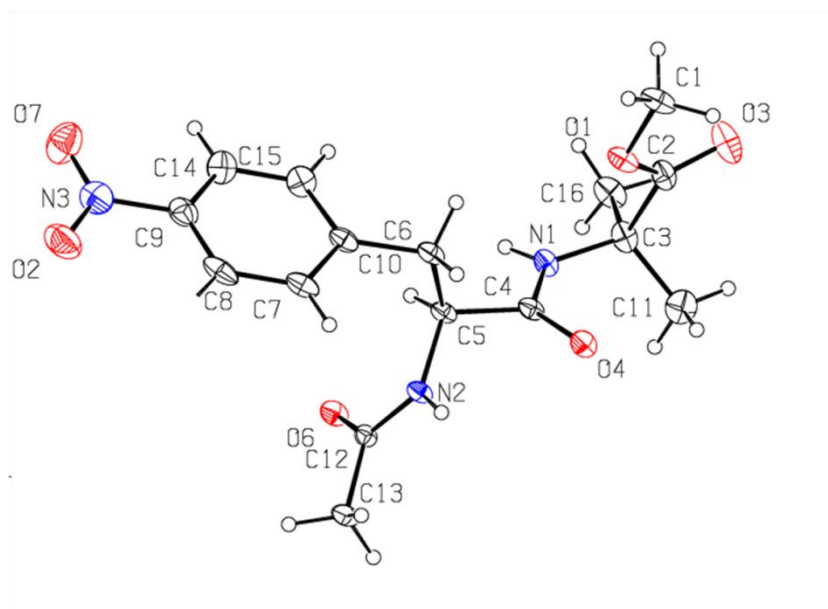


(a)

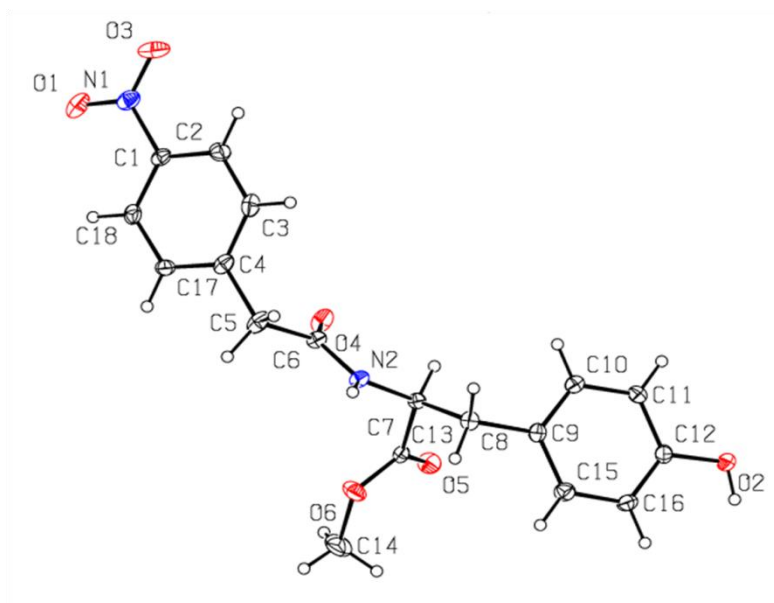


(b)

ESI Fig. 1: IR spectra of (a) peptide 1 and (b) peptide 2.

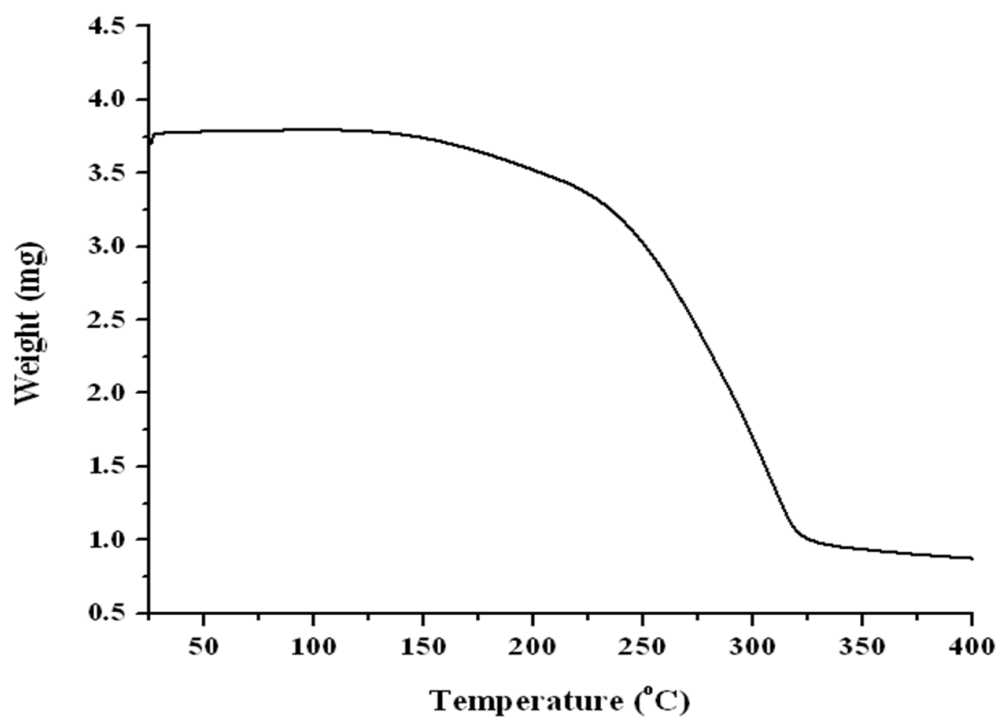


(a)

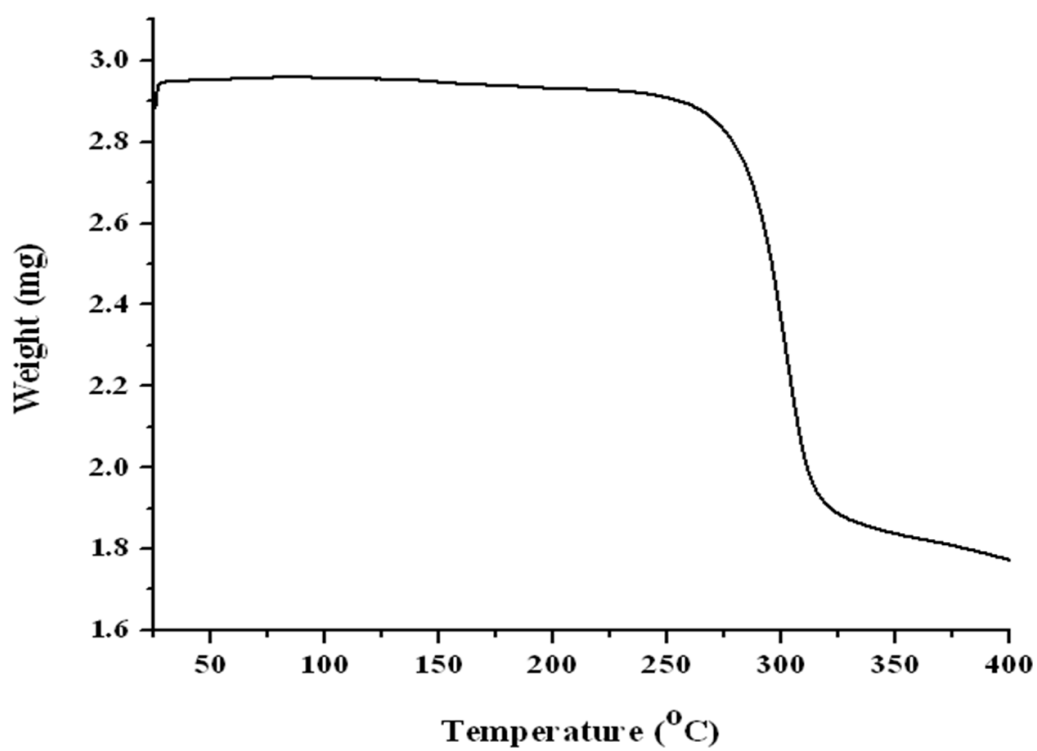


(b)

ESI Fig. 2: ORTEP diagram of (a) peptide 1 and (b) peptide 2 showing the atomic numbering scheme. Ellipsoids are drawn at the 50% probability level.

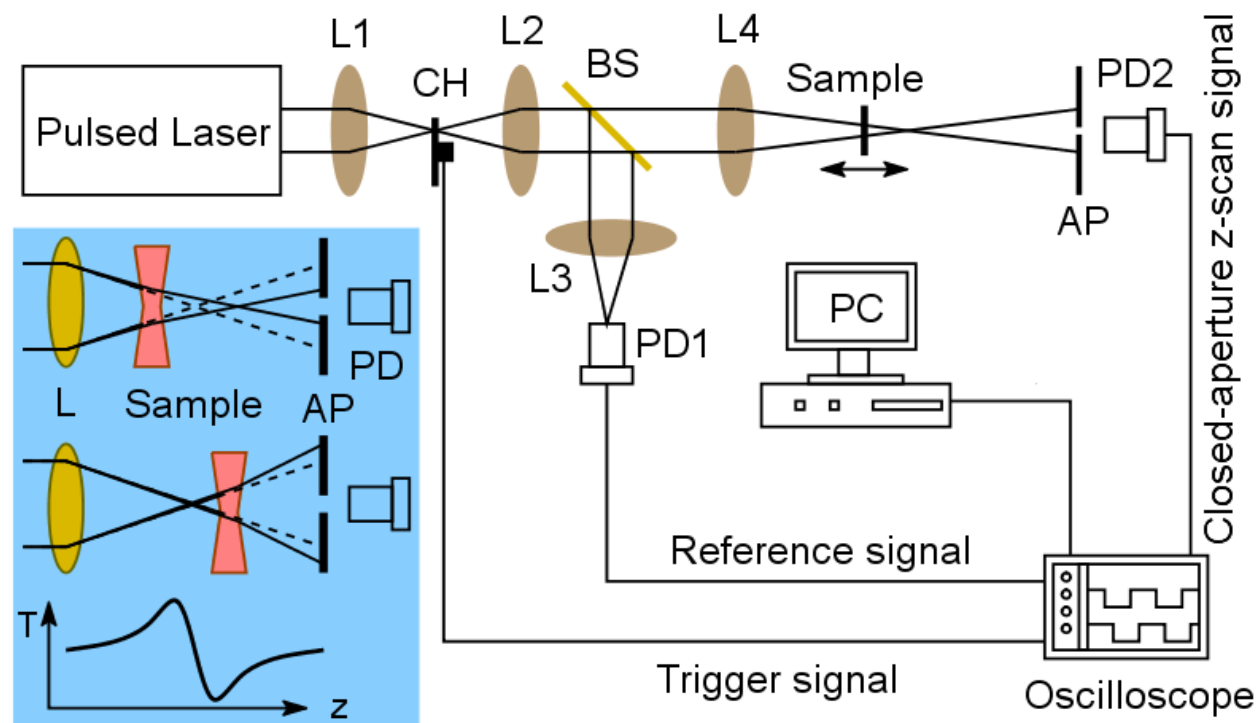


(a)

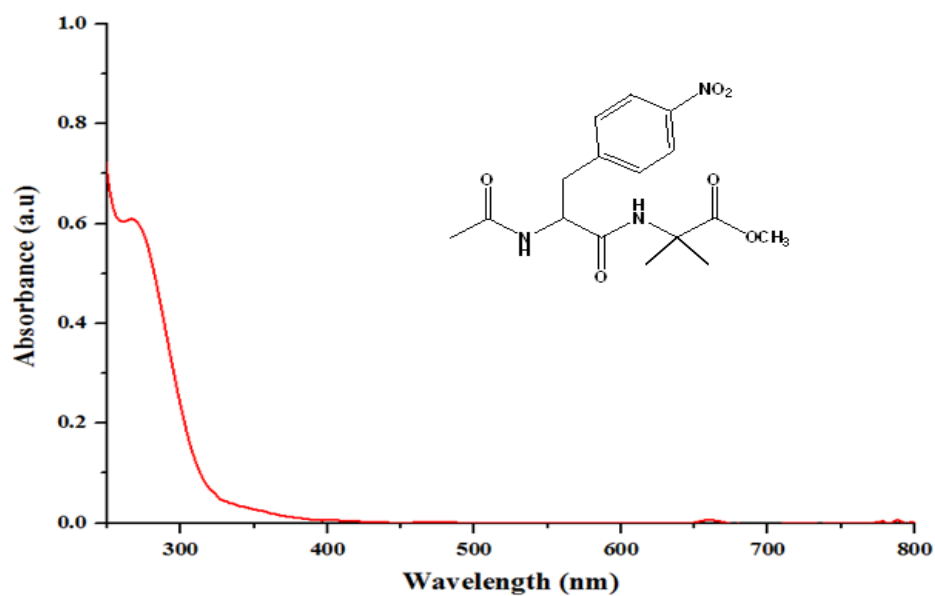


(b)

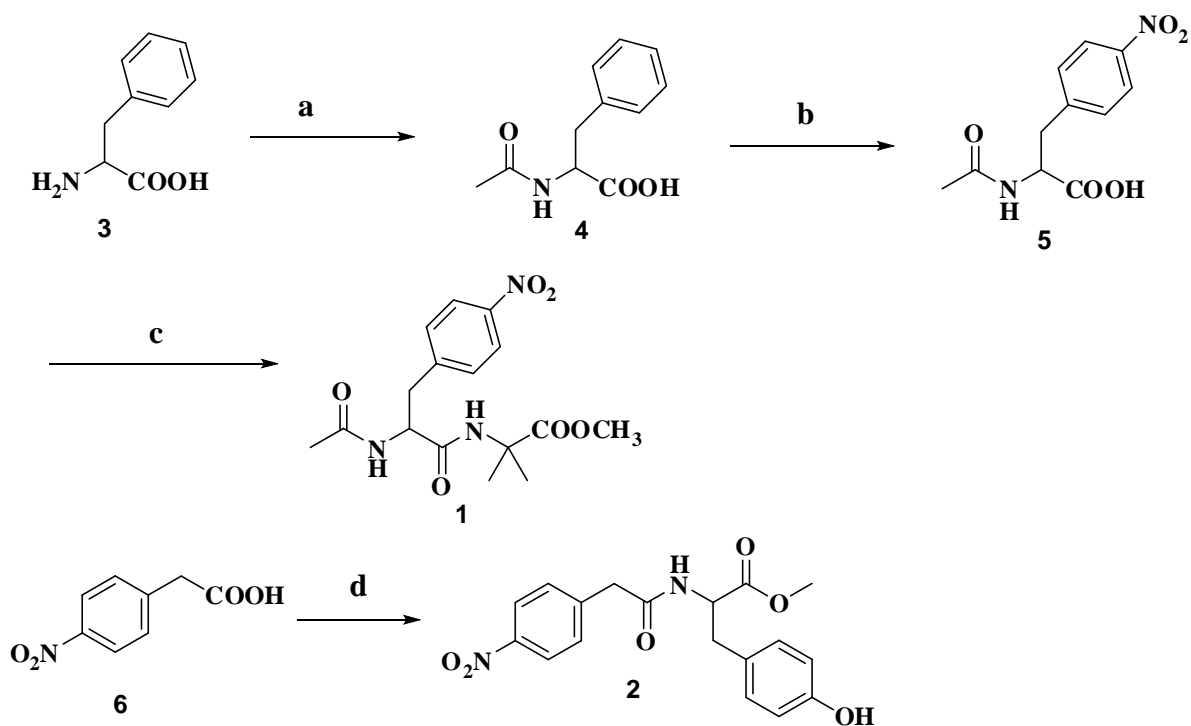
ESI Fig. 3: TGA-DTH spectra of (a) peptide 1 and (b) peptide 2.



ESI Fig. 4: Schematic of Z-scan setup.



ESI Fig. 5: UV- visible spectra of peptide 1.



Scheme 1: Reactions and conditions: a) CH_3COCl , pyridine, 8h, 84%, b) conc. H_2SO_4 , conc. HNO_3 , 82%, c) dry DCM, H-Aib-COOCH₃, DCC, HOBT, 0 °C, 80%, d) dry DCM, H-Tyr-COOCH₃, DCC, HOBT, 0 °C, 85%.

Fig. S1: Schematic presentation of synthesis of peptide 1 and 2.

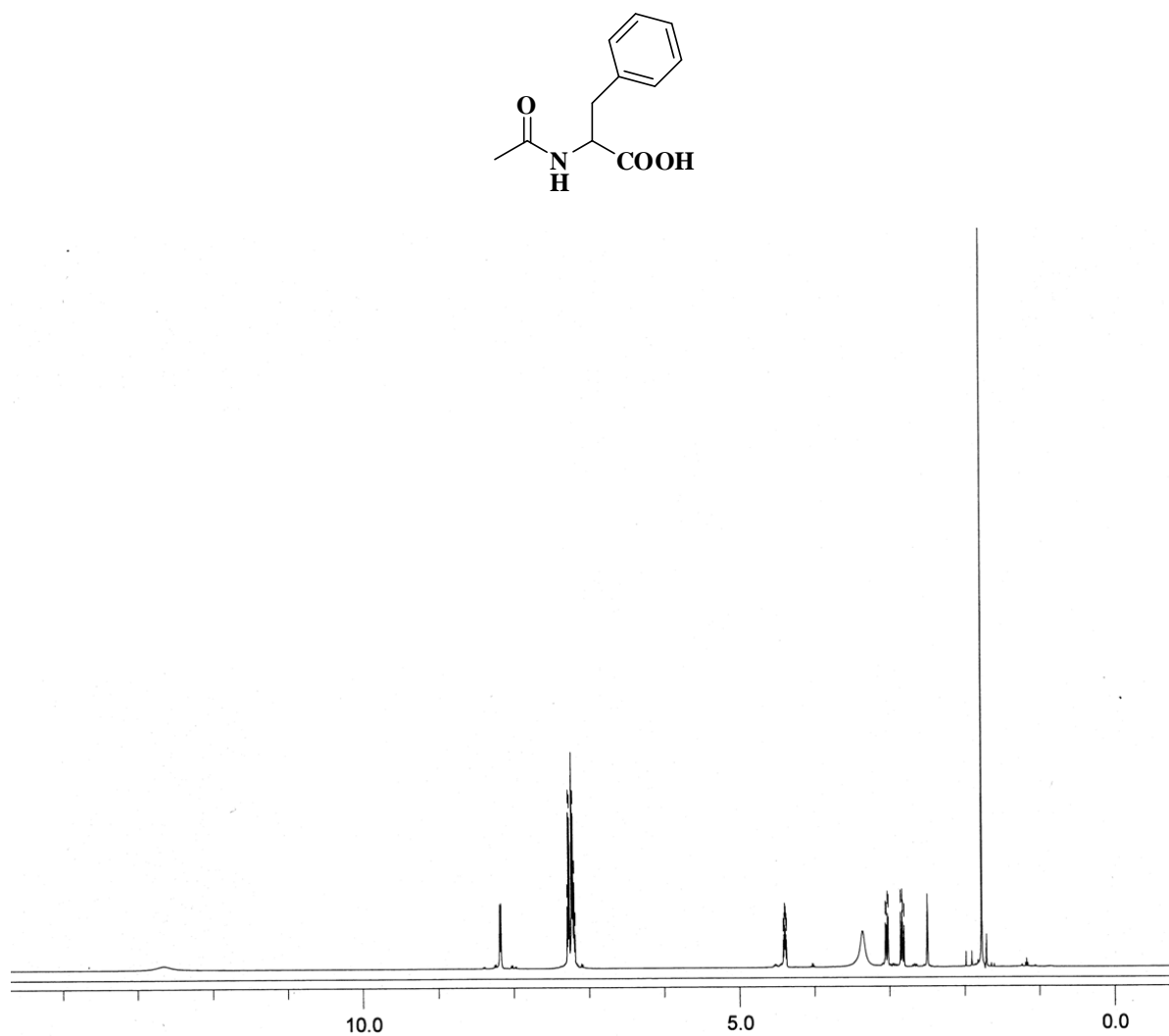


Fig. S2: ¹H NMR (500 MHz, DMSO-*d*₆, δppm) spectrum of compound **4**.

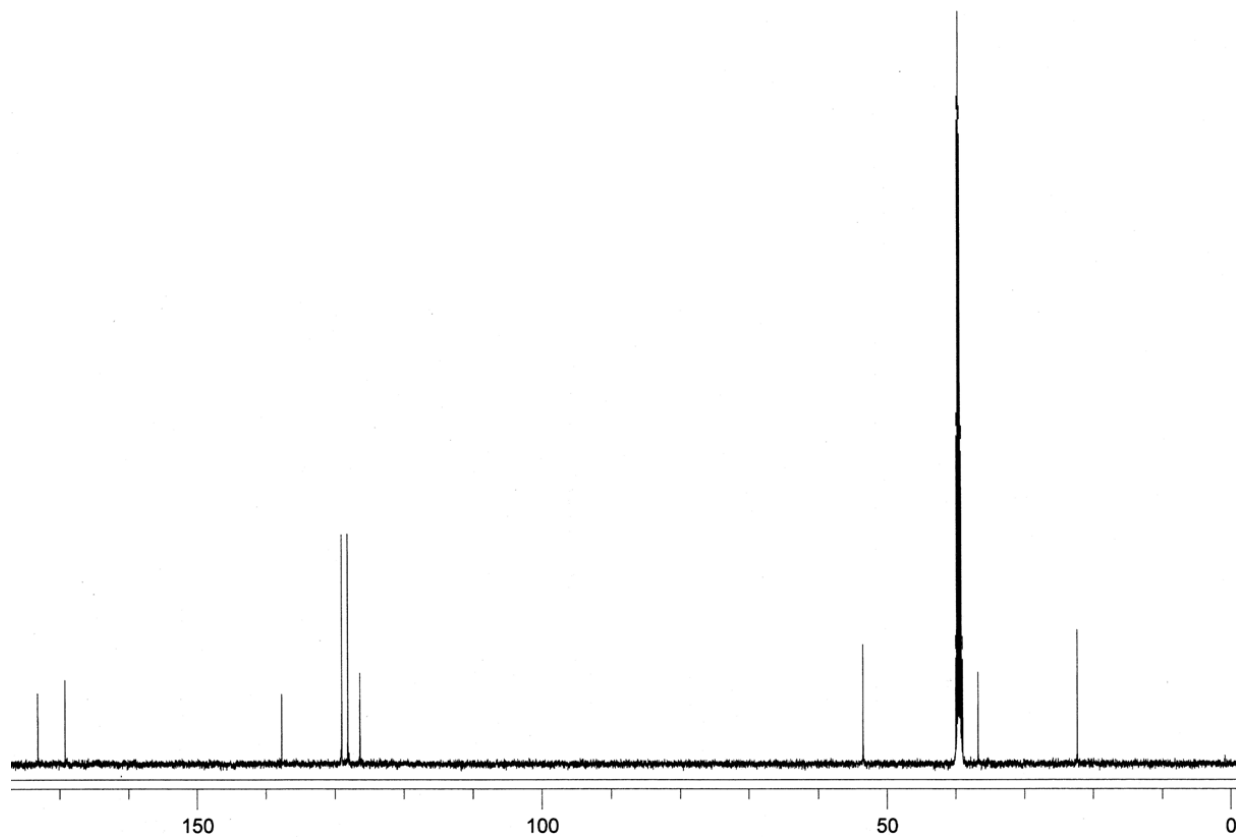
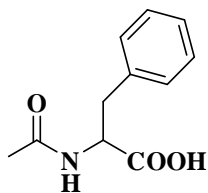


Fig. S3: ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$, δppm) spectrum of compound **4**.

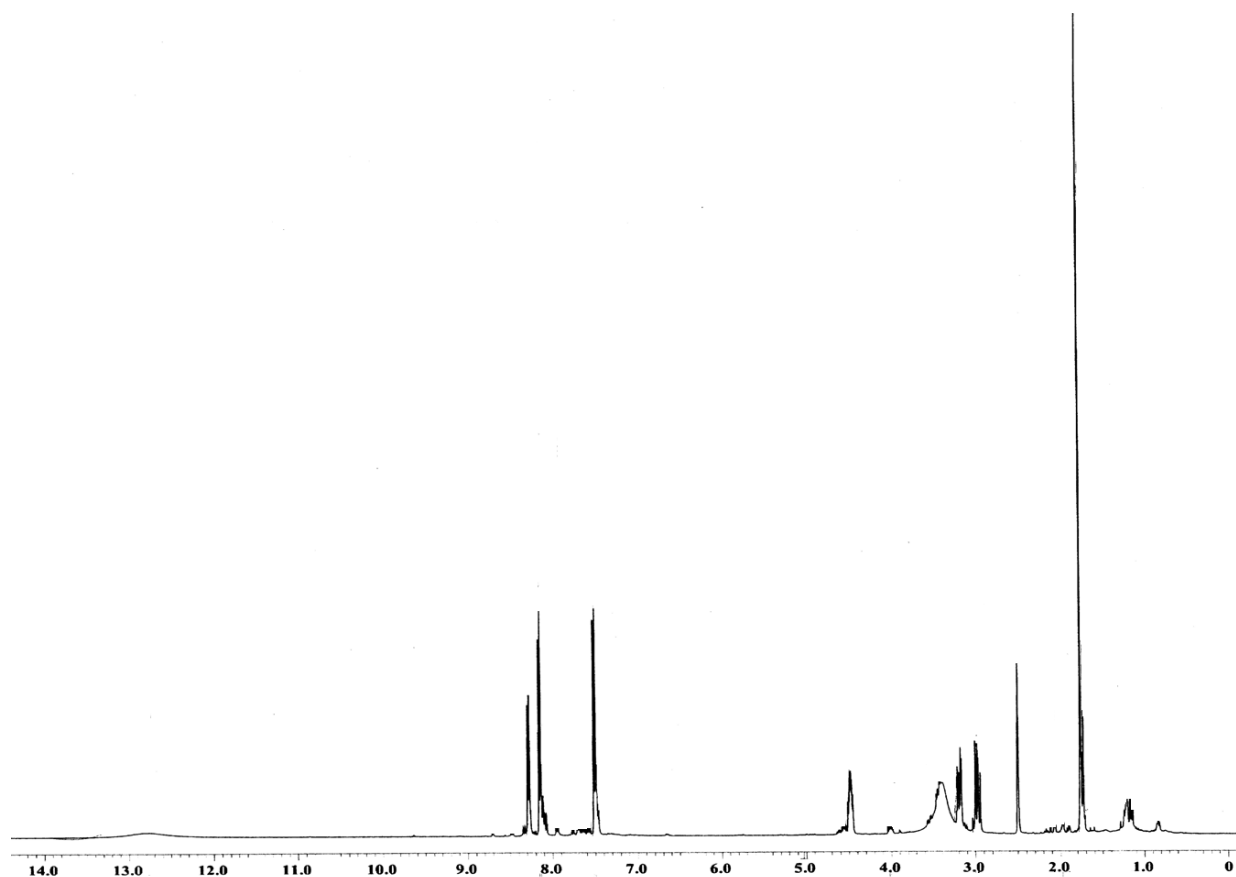
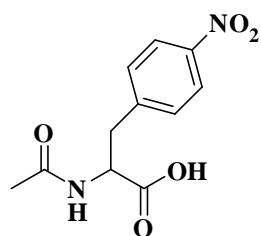


Fig. S4: ^1H NMR (400 MHz, $\text{DMSO}-d_6$, δppm) spectrum of compound **5**.

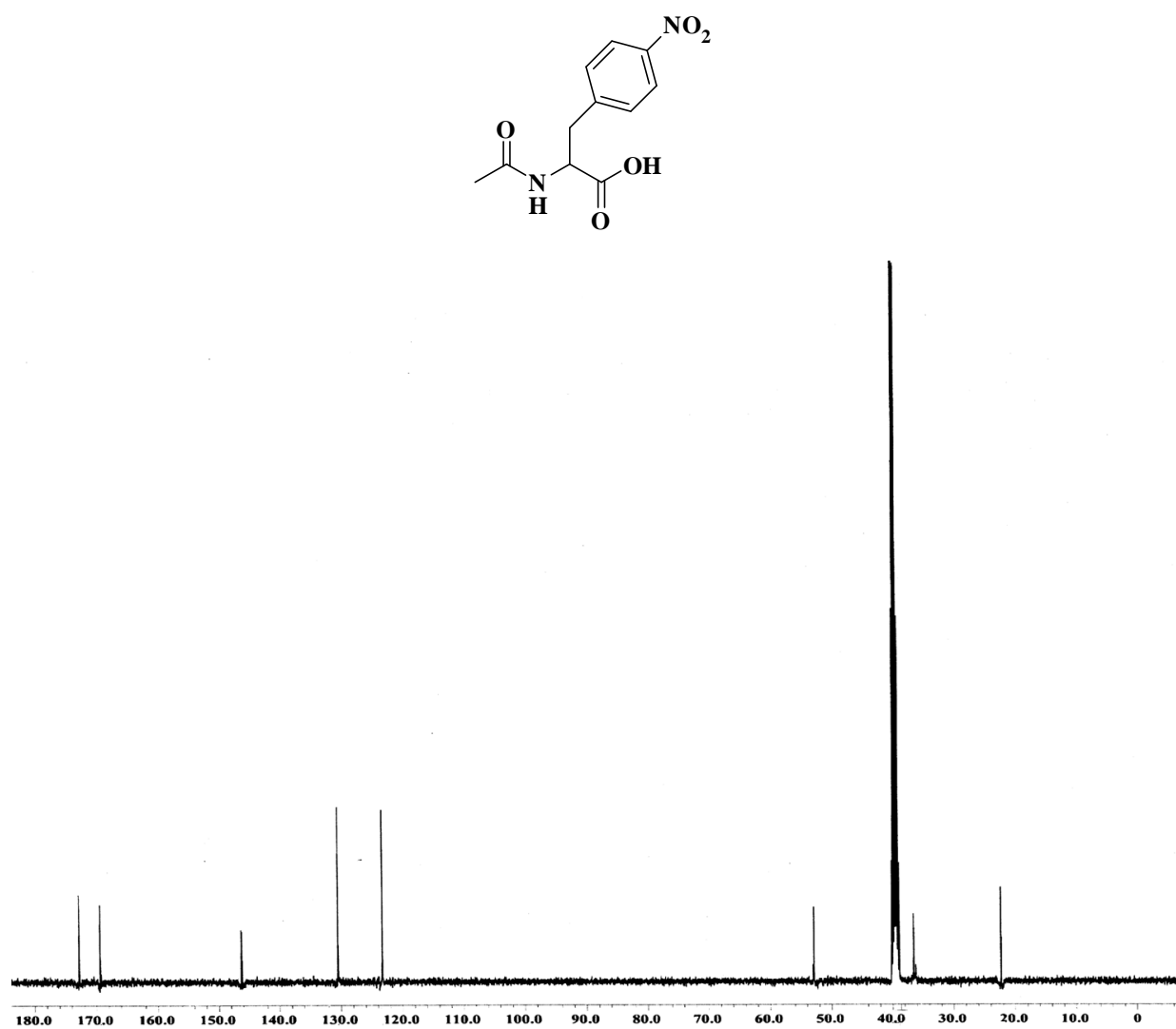


Fig. S5: ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$, δppm) spectrum of compound 5.

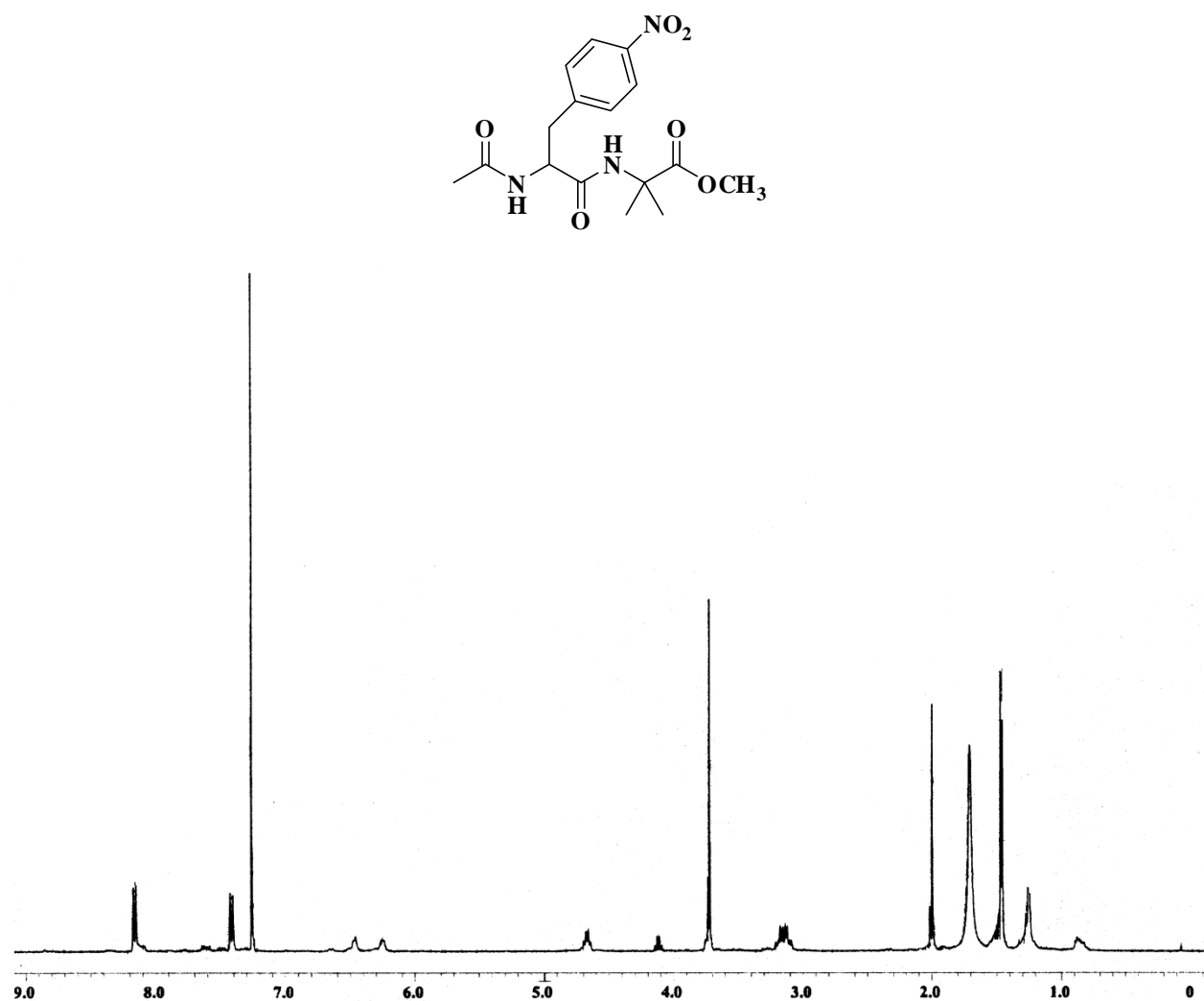


Fig. S6: ^1H NMR (400 MHz, CDCl_3 , δppm) spectrum of peptide **1**.

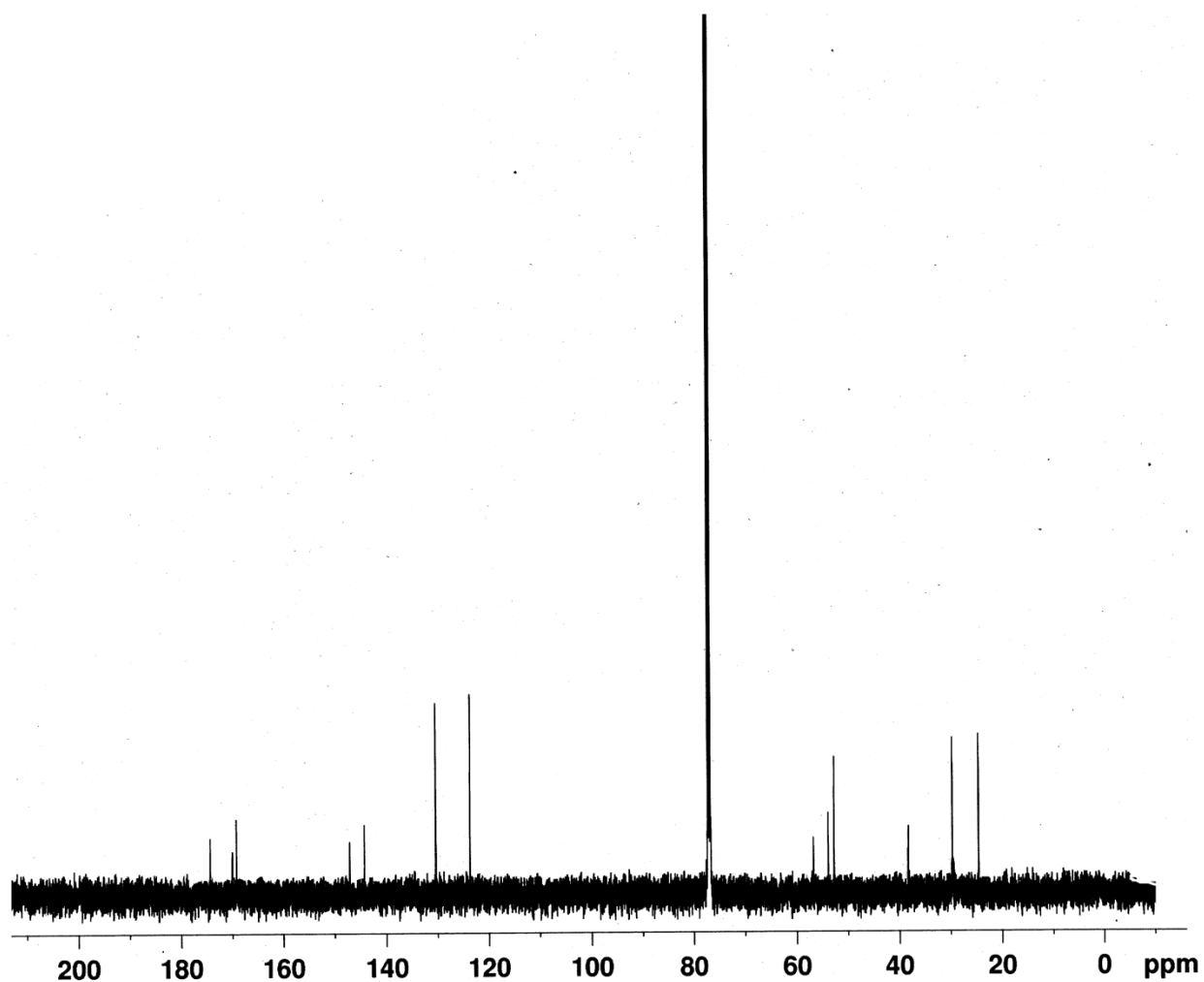
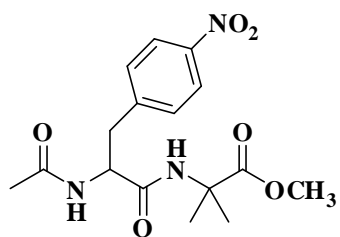


Fig. S7: ^1H NMR (100 MHz, CDCl_3 , δppm) spectrum of peptide **1**.

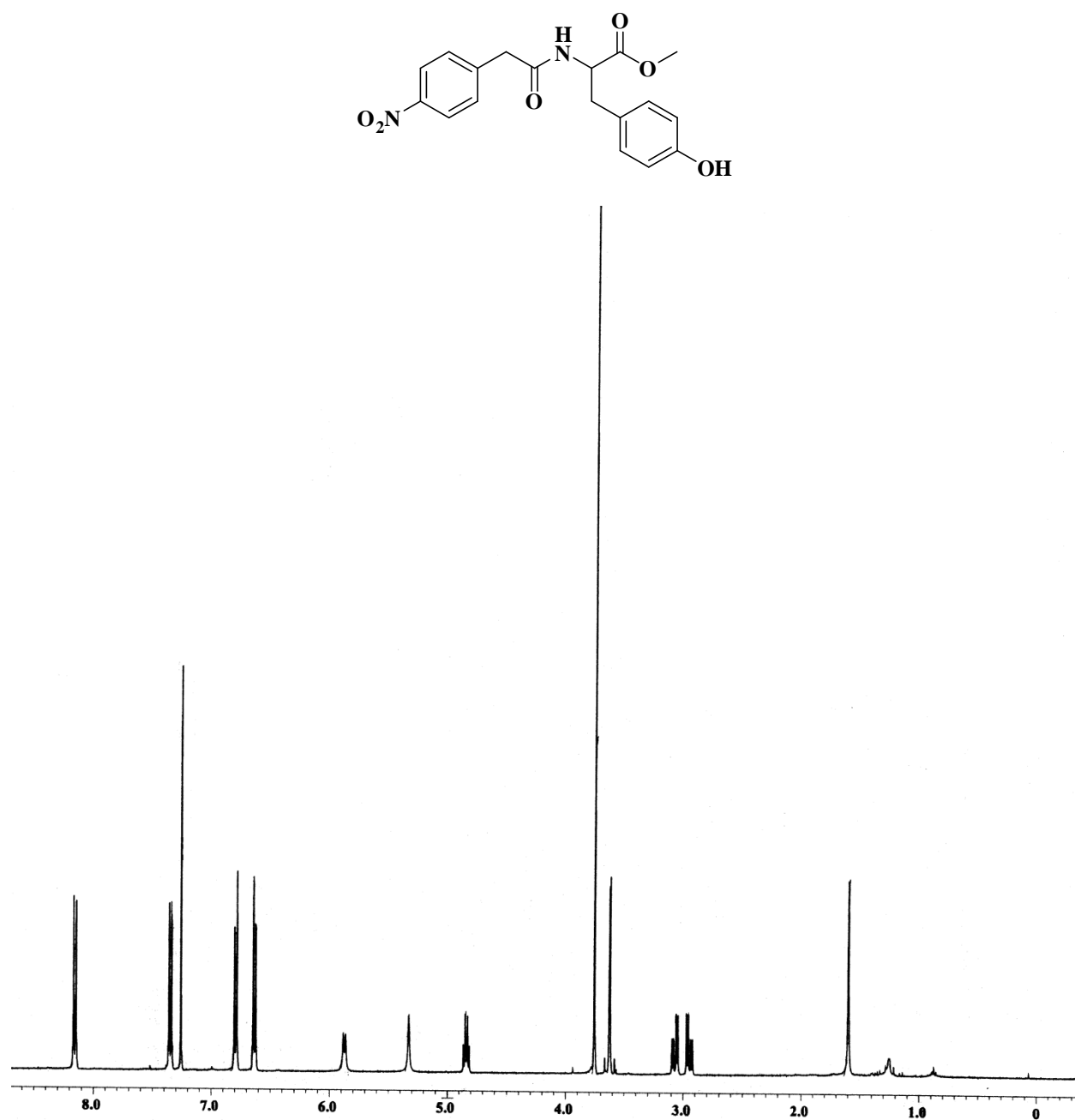


Fig. S8: ^1H NMR (500 MHz, CDCl_3 , δ ppm) spectrum of peptide 2.

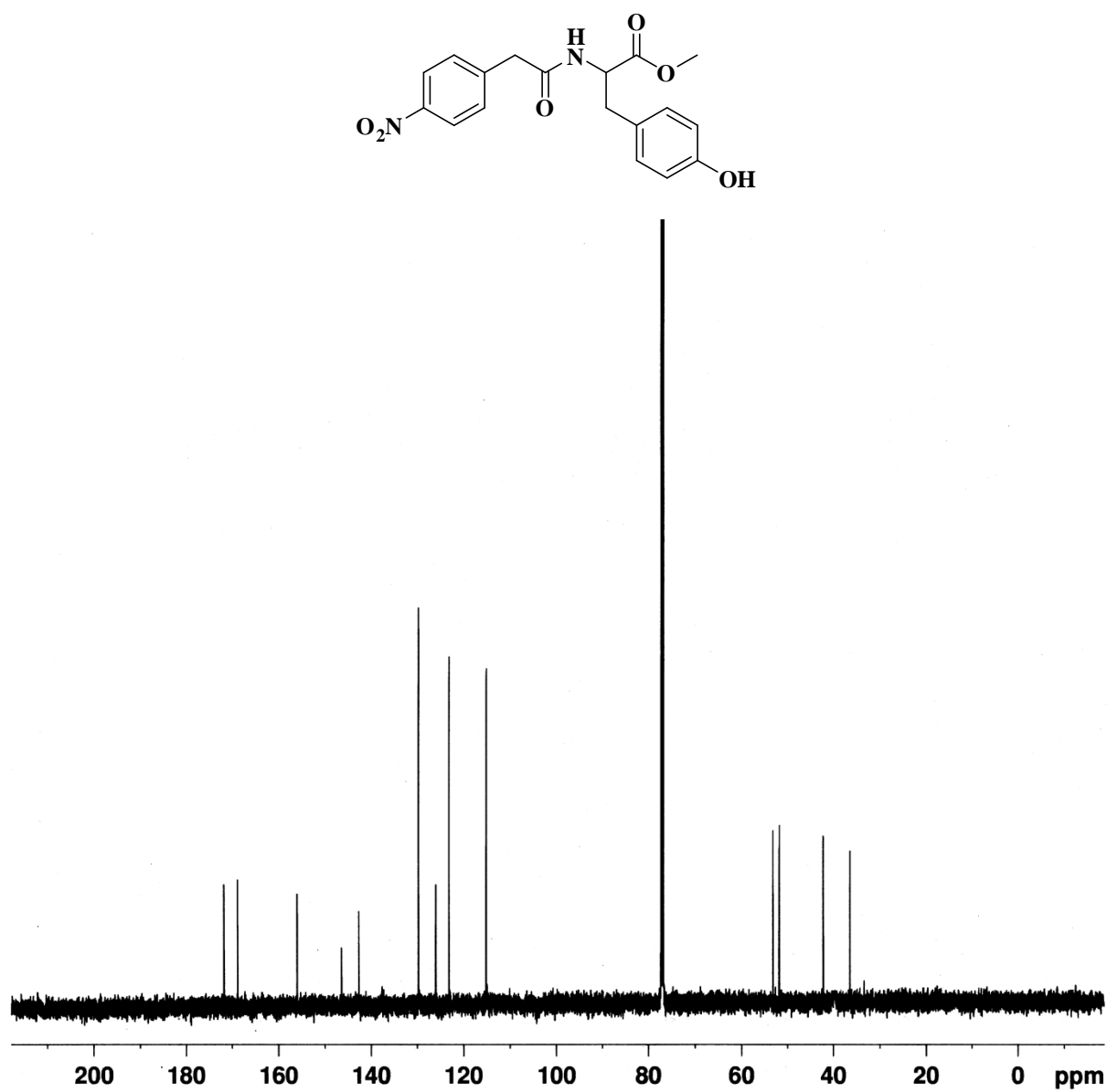


Fig. S9: ¹³C NMR (125 MHz, CDCl₃, δppm) spectrum of peptide 2.

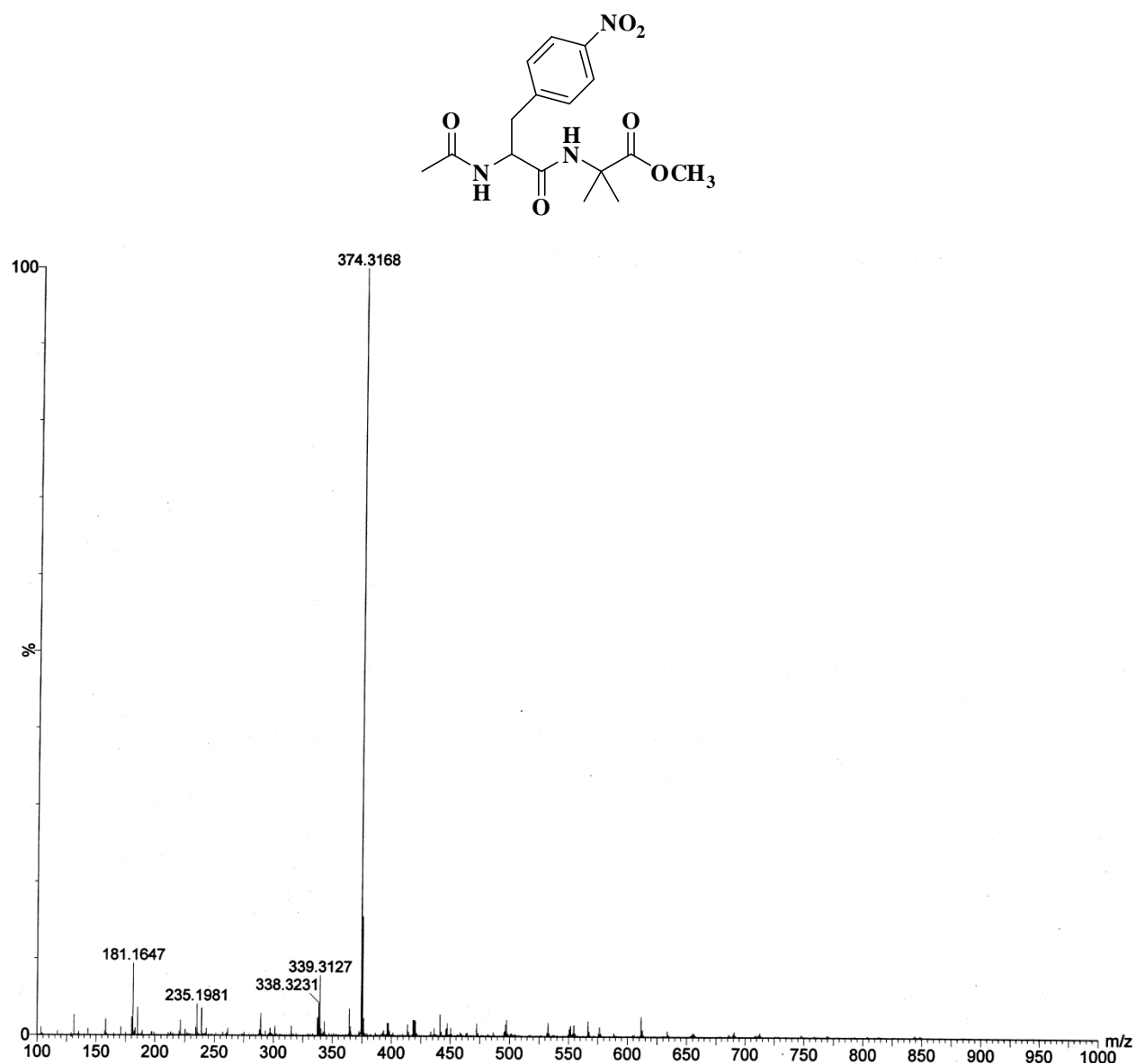


Fig. S10: Mass spectrum of peptide 1.

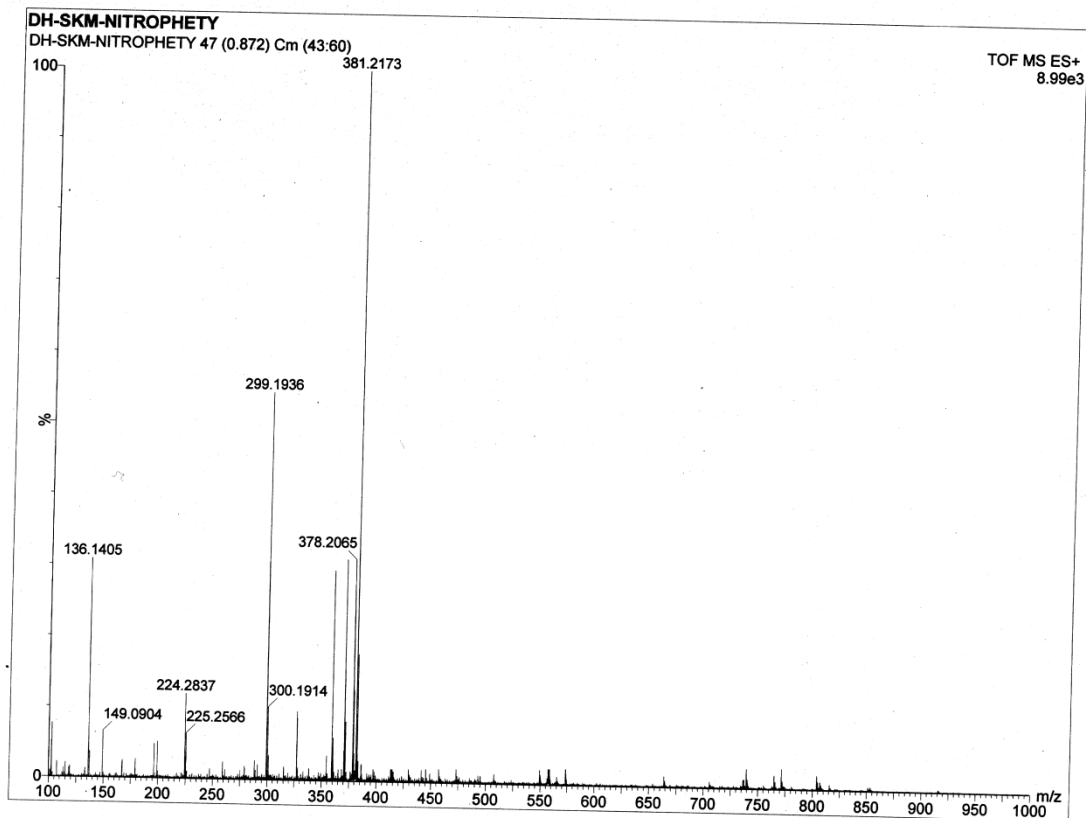
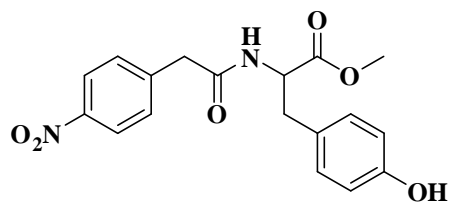


Fig. S11: Mass spectrum of peptide 2.