Design, Synthesis, and Characterisation of Glyoxylamide-Based Short Peptides as Self-Assembled Gels

Vina R. Aldilla[a], Shashidhar Nizalapur[a], Adam Martin[a*], Chris E. Marjo[b], Anne Rich[b], Eugene Yee[a], Panthipa Suwannakot[a], David Black[a], Pall Thordarson[a*], Naresh Kumar[a*]

[a]. School of Chemistry, UNSW Australia, Sydney, NSW 2052, Australia

[b]. Mark Wainwright Analytical Centre, UNSW Australia, Sydney NSW 2052, Australia

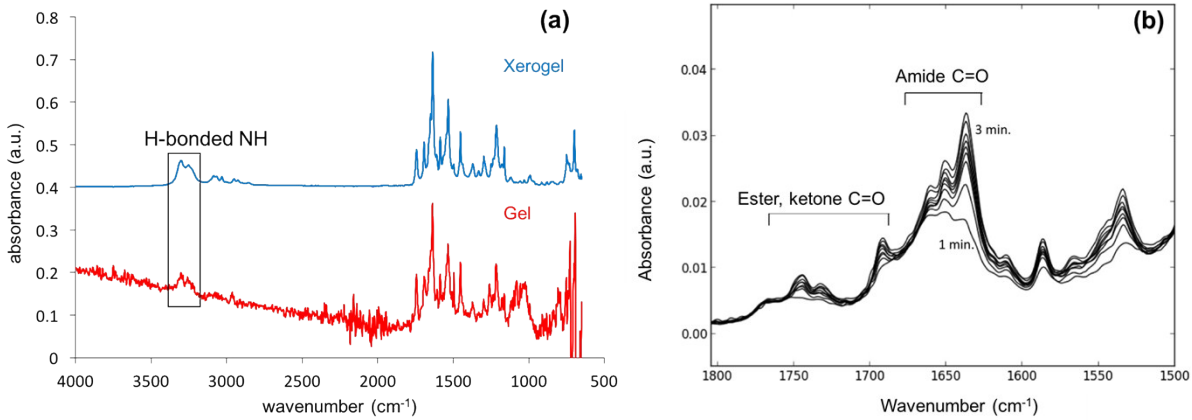

Figure S 1: (a) Stackplot of absorbance ATR-FTIR spectra of **5a** in their xerogel-form and gel-form, with toluene solvent subtracted, showing hydrogen-bonded NH peaks in both phases at 3400-3200 cm^{-1}. ATR-FTIR spectral overlay of carbonyl peak region during the first 3 minutes of the experiment in 2-propanol, with characteristic carbonyl regions indicated by brackets. Spectra are displayed in absorbance mode with an x-axis in wavenumber (cm^{-1}).

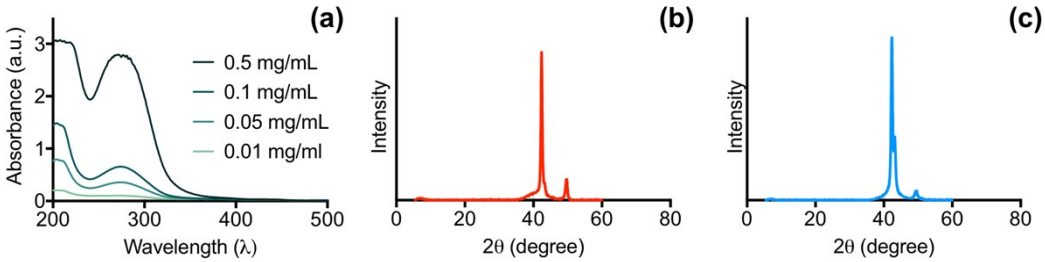

Figure S 2 : (a) UV/Vis spectra of **5a** in 2-propanol with different concentrations. Powder X-Ray diffraction of **5a** in their (b) gel-form (c) xerogel form

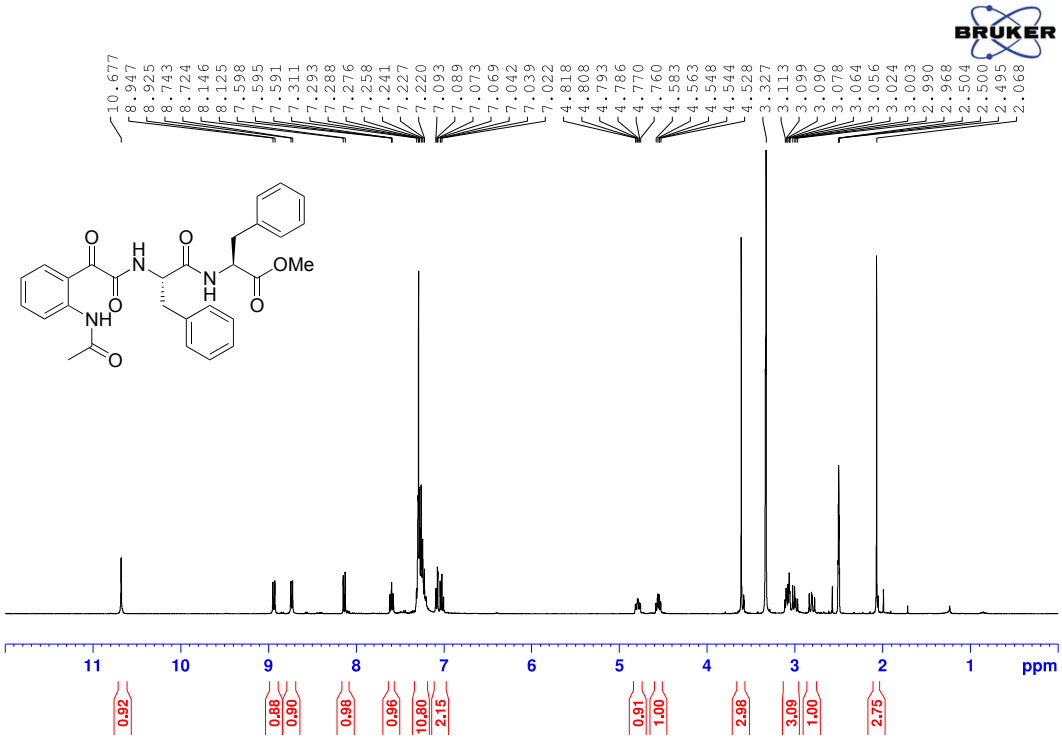

Figure S 3 :[1]H NMR spectrum of Methyl (2-(2-acetamidophenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5a.**

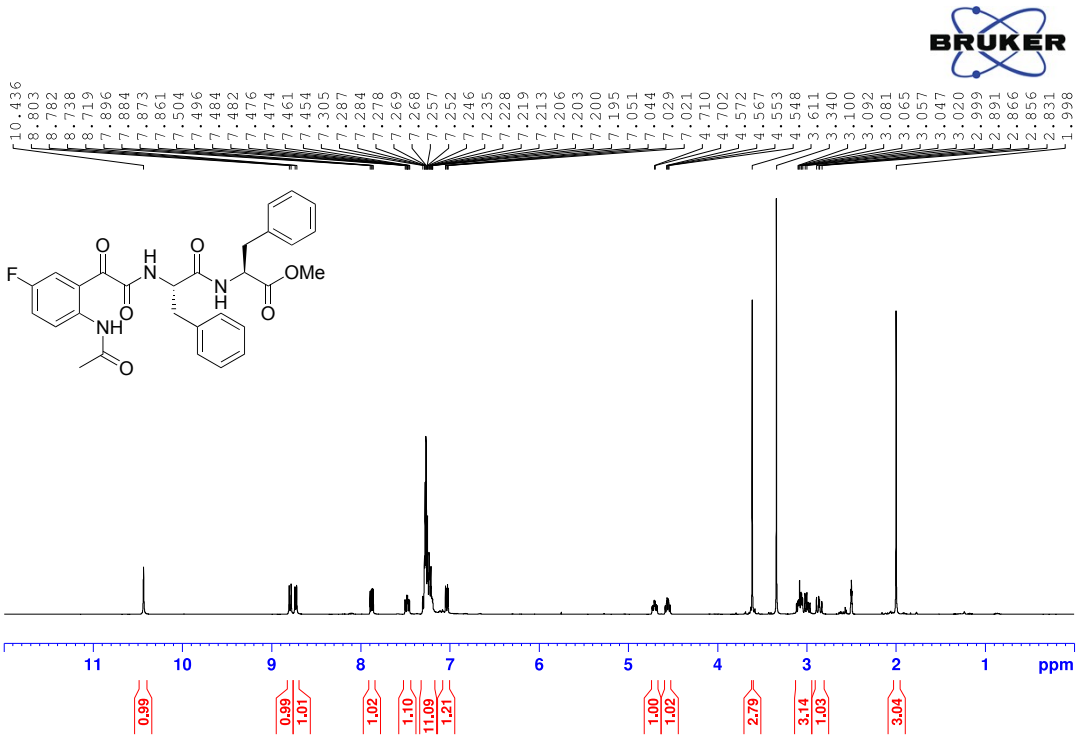

Figure S 4:[1]H NMR spectrum of Methyl (2-(2-acetamido-5-fluorophenyl)-2-oxoacetyl)-L- phenylalanyl-L-phenylalaninate **5b.**

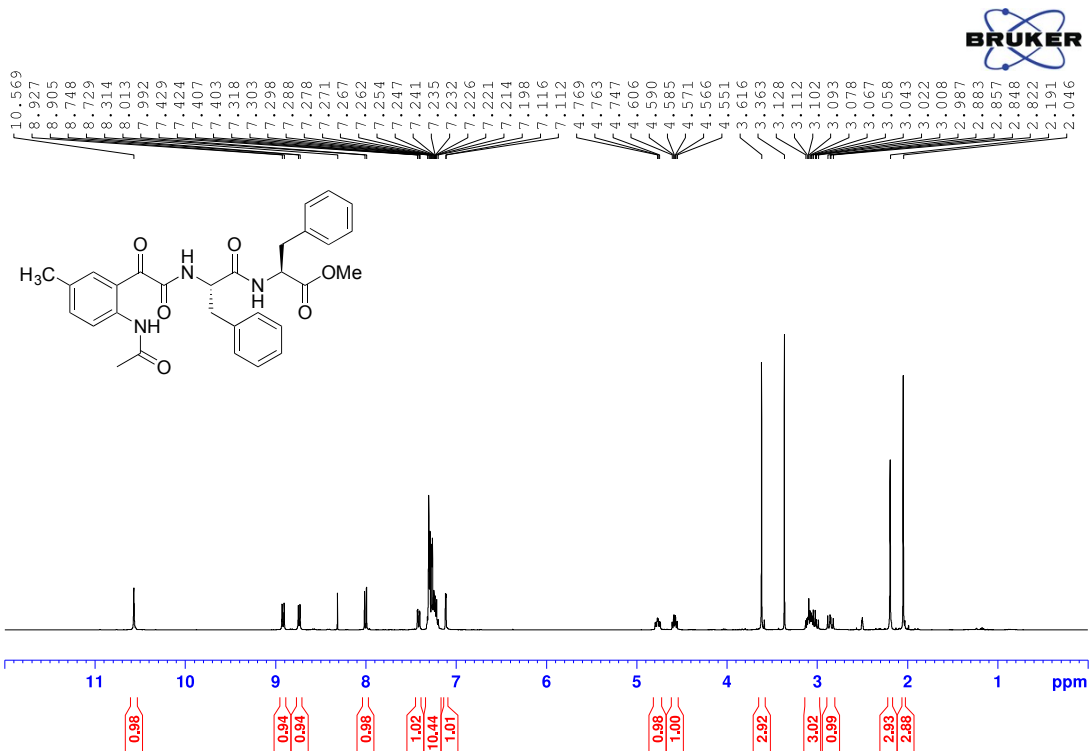

Figure S 5:[1]H NMR spectrum of methyl (2-(2-acetamido-5-methylphenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5c**.

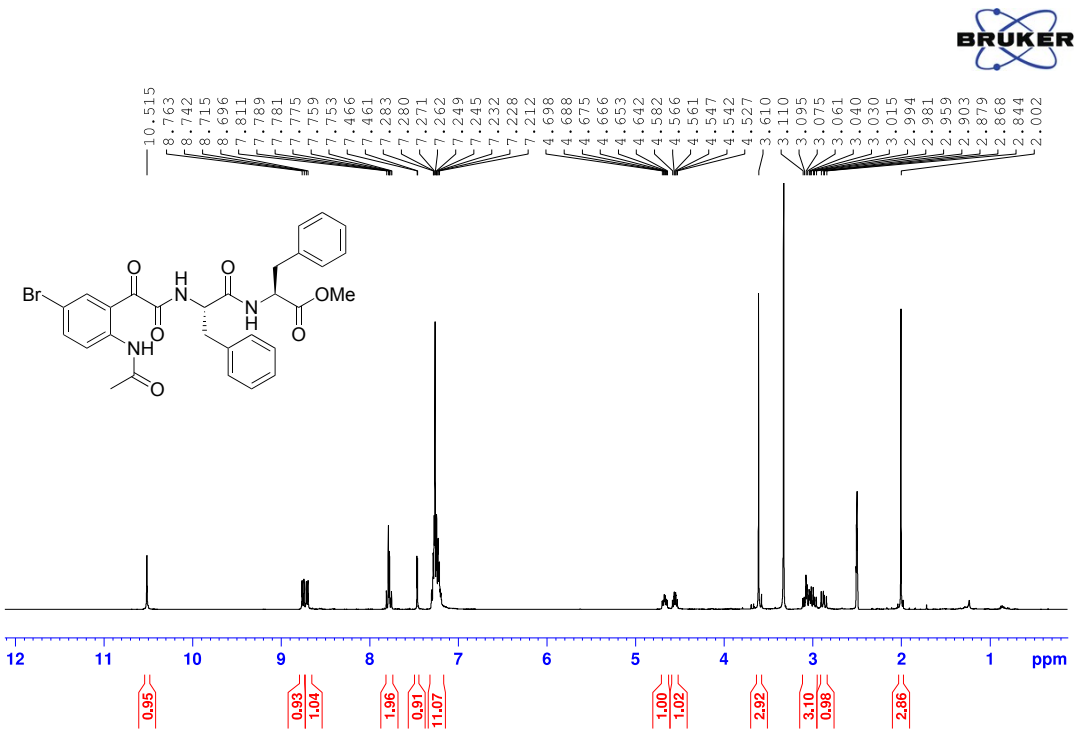

Figure S 6: [1]H NMR spectrum of methyl (2-(2-acetamido-5-bromophenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5d.**

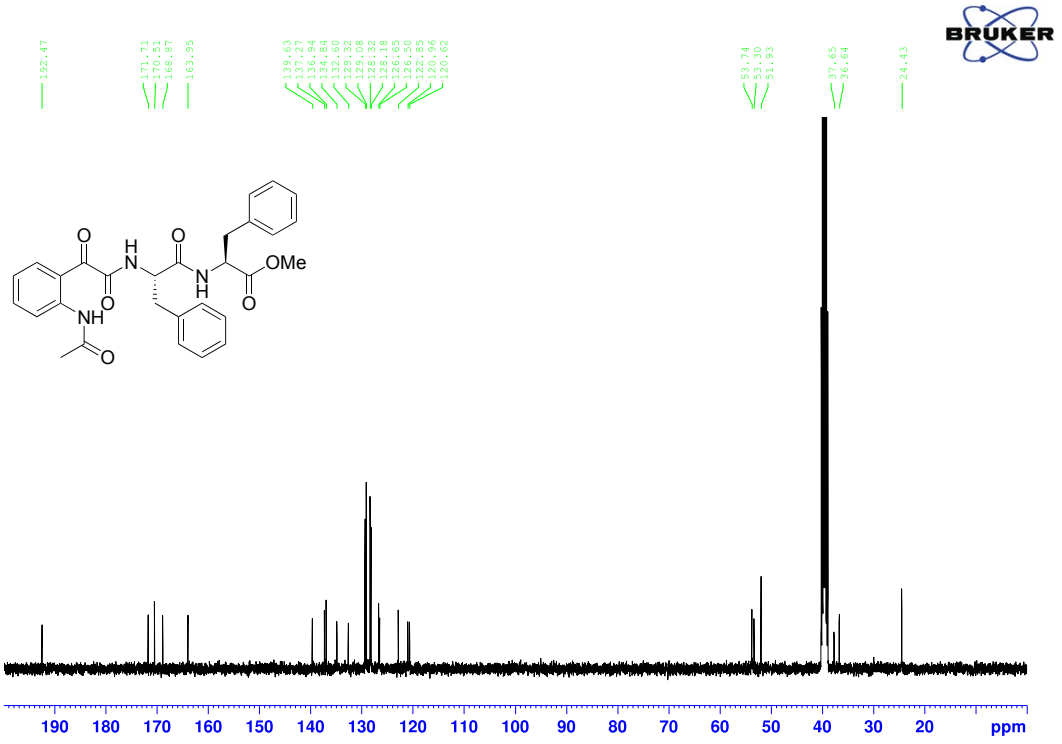

Figure S 7:[13]C NMR spectrum of Methyl (2-(2-acetamidophenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5a.**

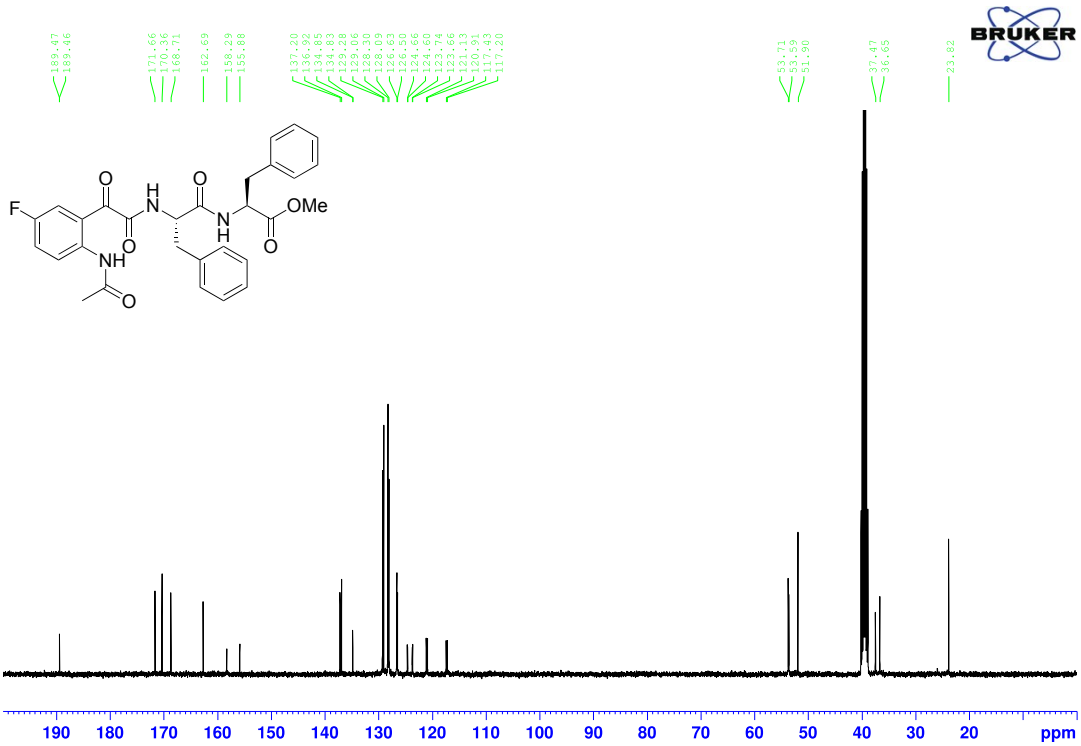

Figure S 8:[13]C NMR spectrum of Methyl (2-(2-acetamido-5-fluorophenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5b.**

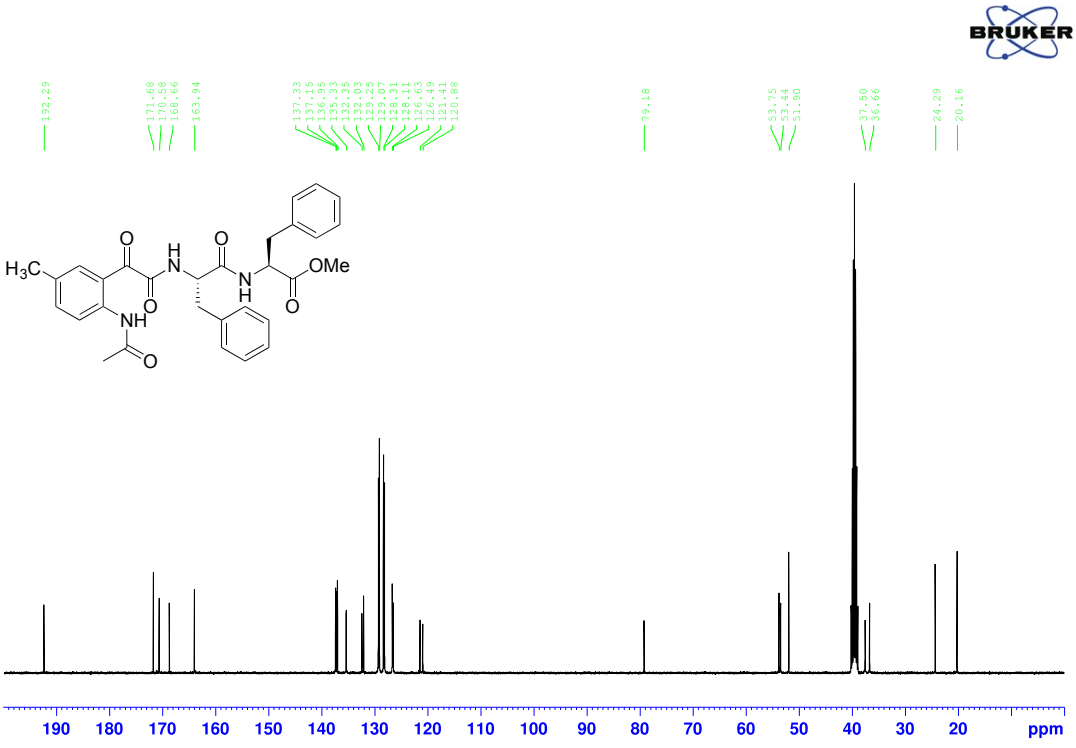

Figure S 9 : ^{13}C NMR spectrum of methyl (2-(2-acetamido-5-methylphenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5c**

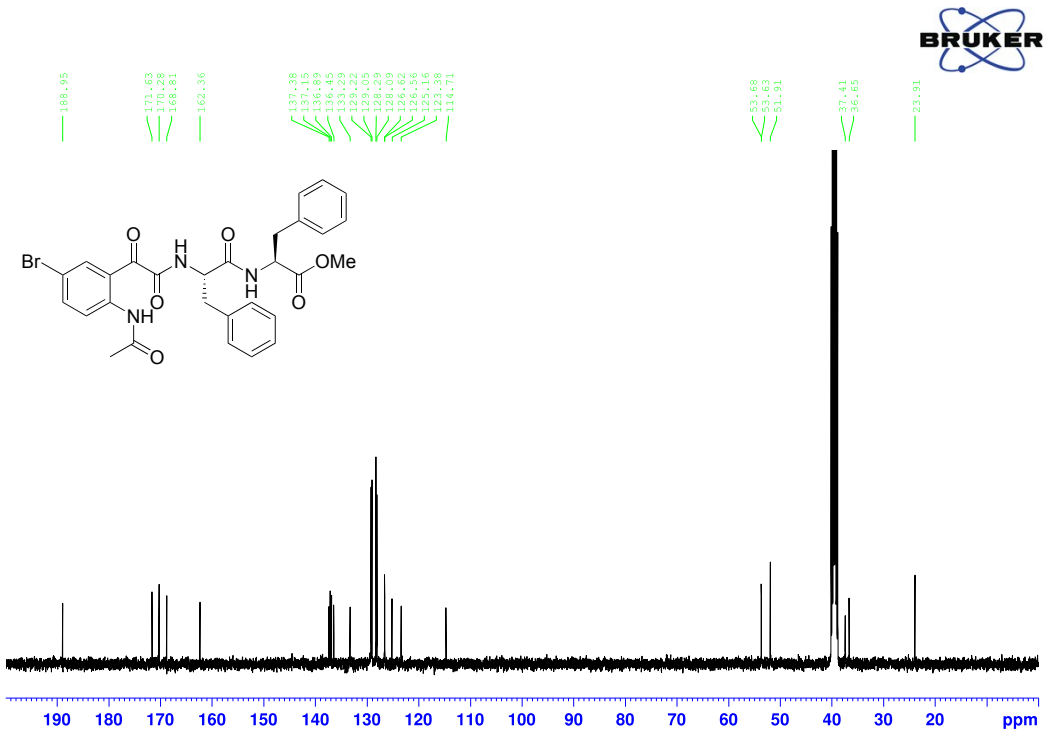

Figure S 10 : ^{13}C NMR spectrum of methyl (2-(2-acetamido-5-bromophenyl)-2-oxoacetyl)-L-phenylalanyl-L-phenylalaninate **5d.**

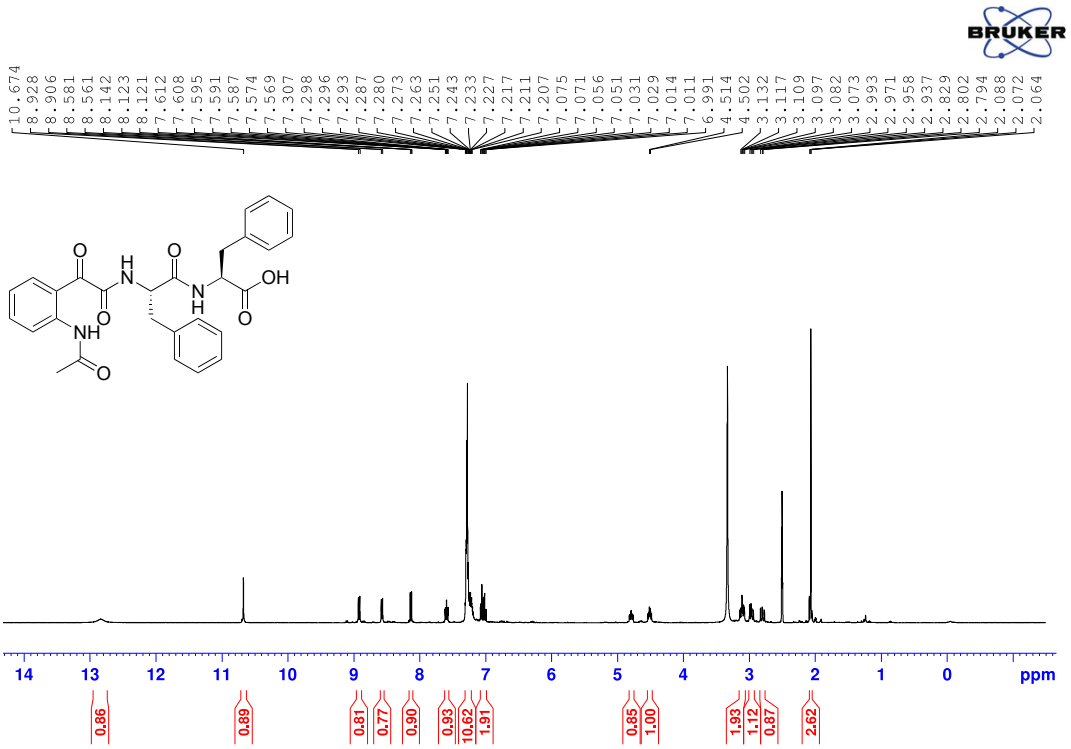

Figure S 11 : ^{1}H NMR spectrum of (2-(2-acetamidophenyl)-2-oxoacetyl)-L-phenylalanyl- L-phenylalanine **6a**.

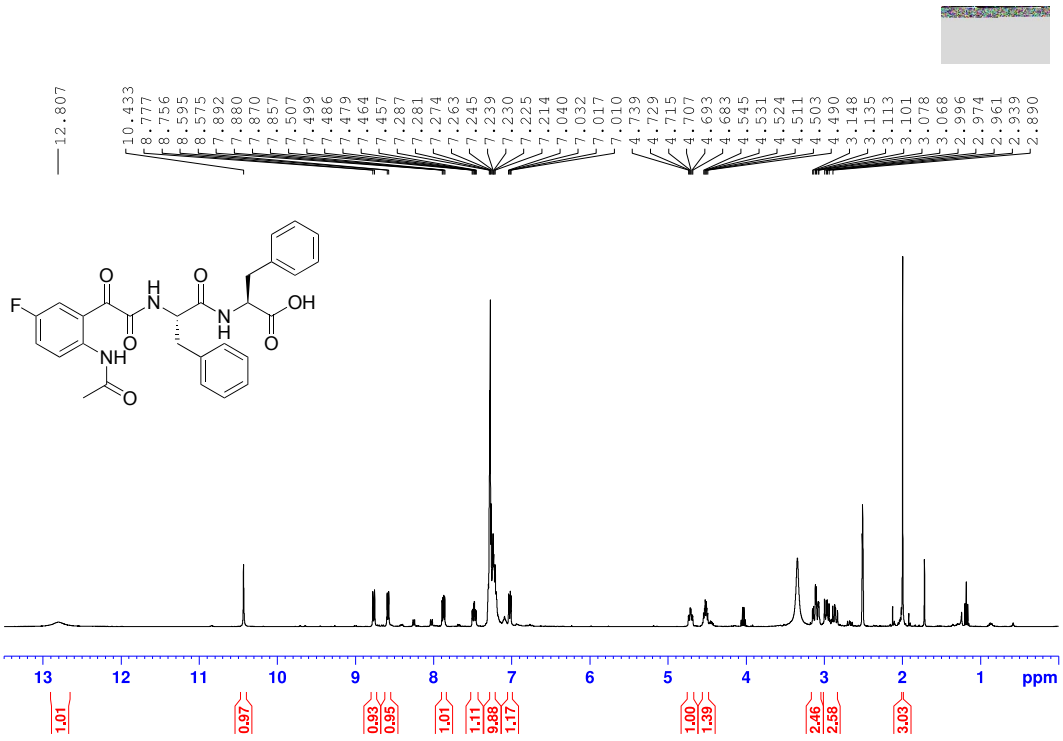

Figure S 12 :^{1}H NMR spectrum of (2-(2-acetamido-5-fluorophenyl)-2-oxoacetyl)-L- phenylalanyl- L-phenylalanine **6b**.

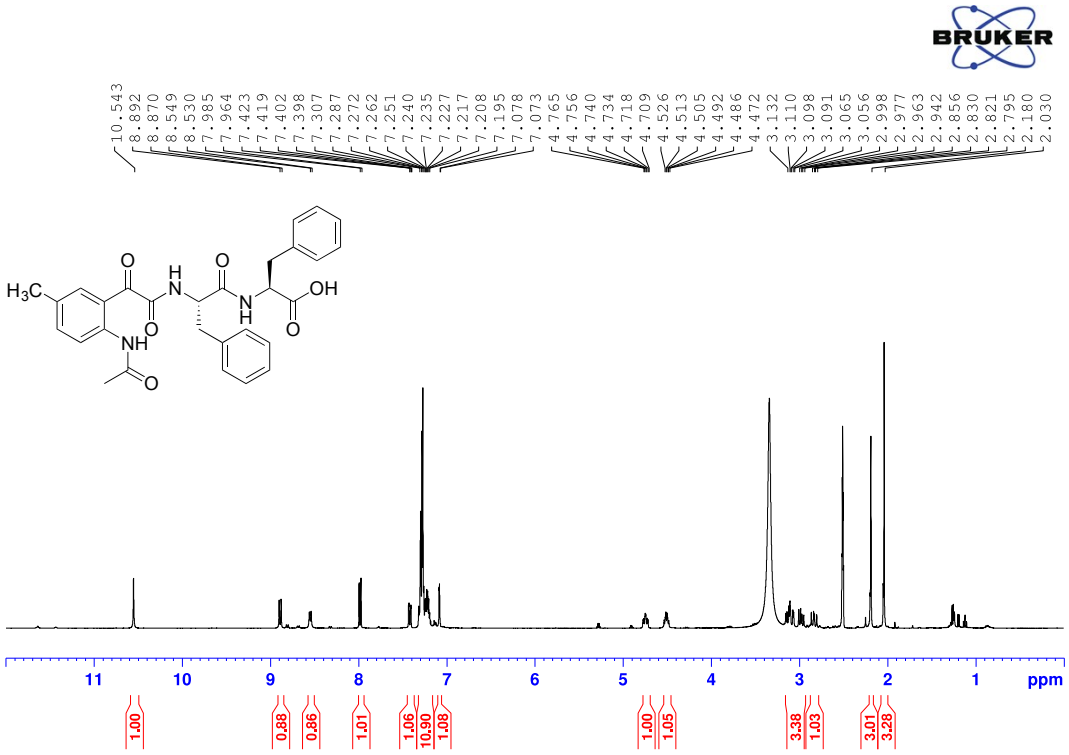

Figure S 13 :[1]H NMR spectrum of (2-(2-acetamido-5-methylphenyl)-2-oxoacetyl)-L-phenylalanyl- L-phenylalanine **6c**.

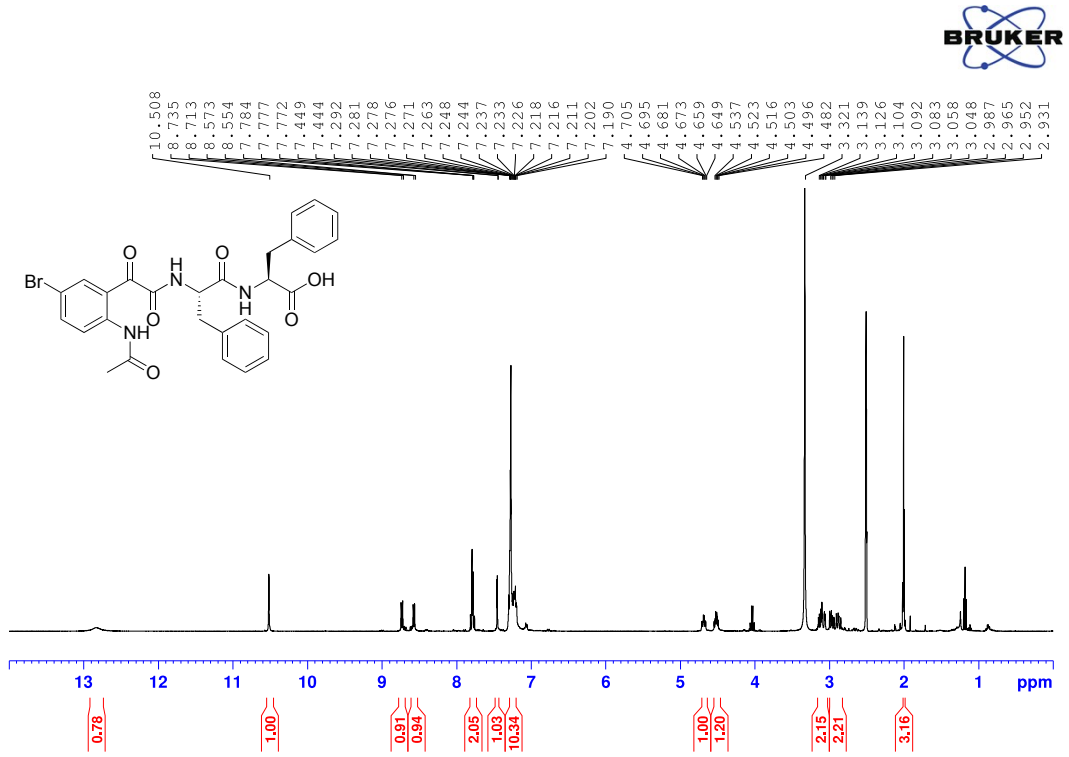

Figure S 14 *:* [1]H NMR spectrum of (2-(2-acetamido-5-bromophenyl)-2-oxoacetyl)-L-phenylalanyl- L-phenylalanine **6d**.

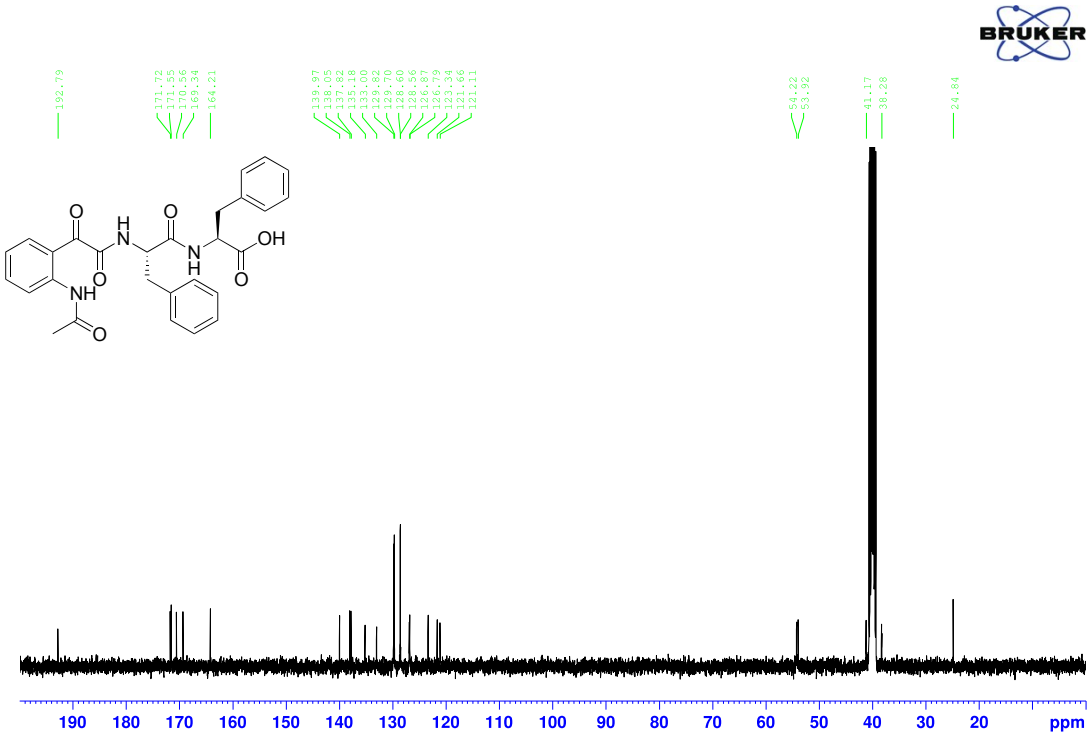

Figure S 15 : ^{13}C NMR spectrum of (2-(2-acetamidophenyl)-2-oxoacetyl)-L-phenylalanyl- L- phenylalanine **6a**.

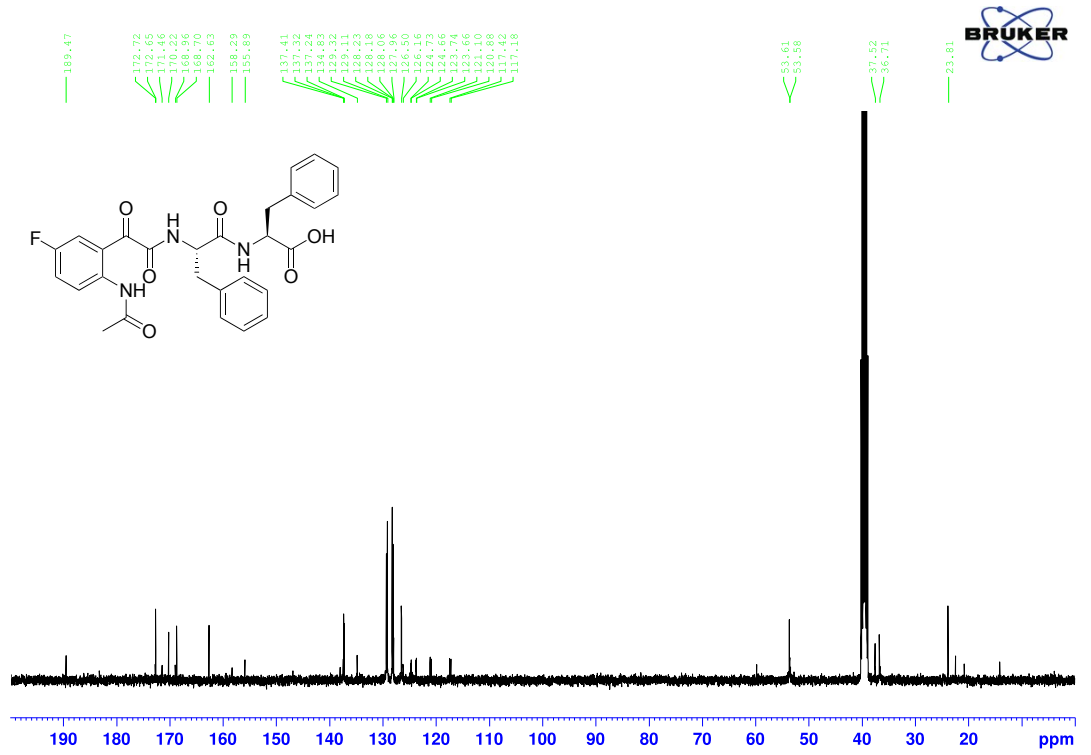

Figure S 16 : ^{13}C NMR spectrum of (2-(2-acetamido-5-fluorophenyl)-2-oxoacetyl)-L-phenylalanyl- L-phenylalanine **6b**.

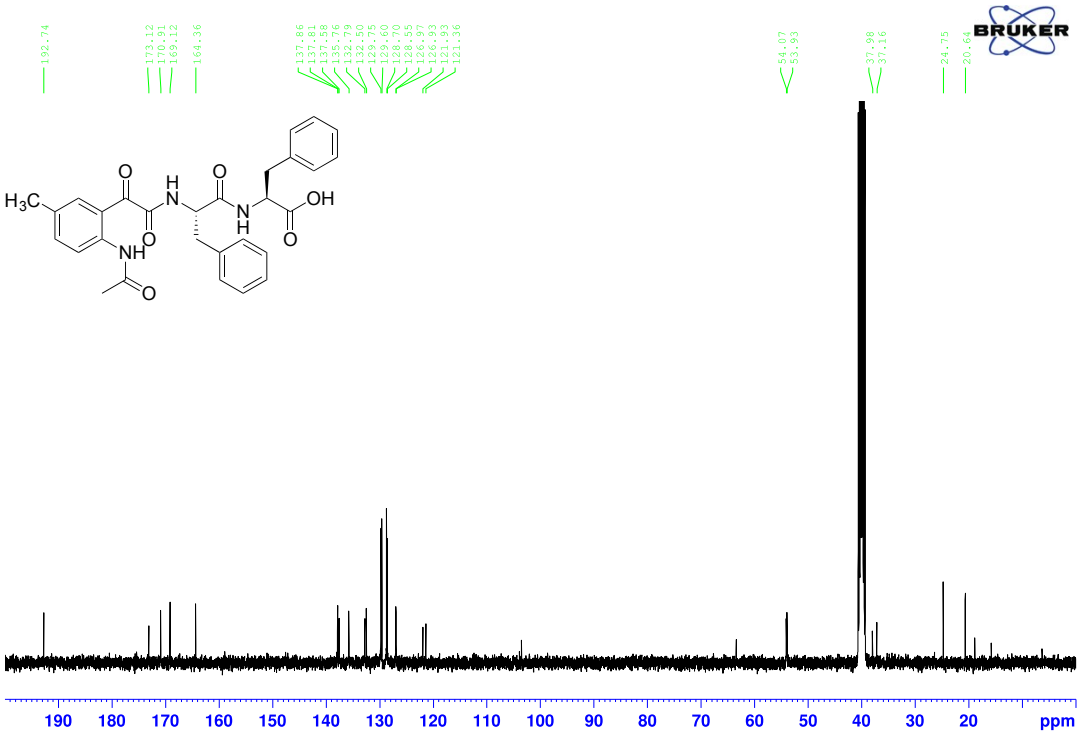

Figure S 17 :^{13}C NMR spectrum of (2-(2-acetamido-5-methylphenyl)-2-oxoacetyl)-L-phenylalanyl- L-phenylalanine **6c**.

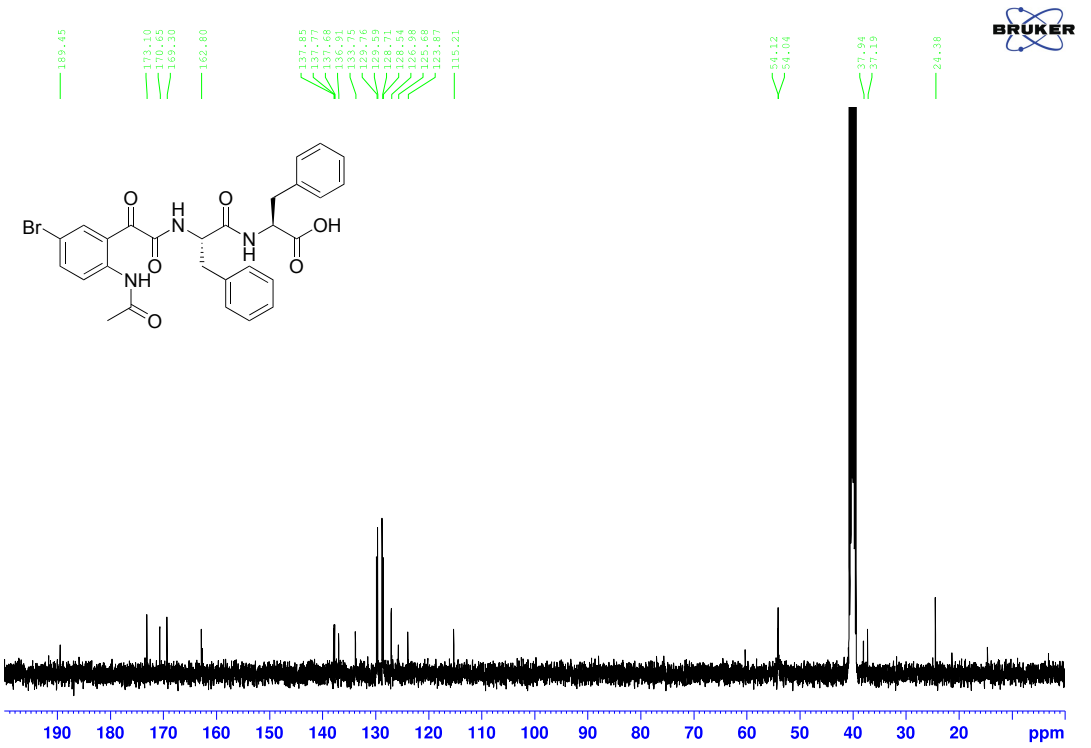

Figure S 18 : ^{13}C NMR spectrum of (2-(2-acetamido-5-bromophenyl)-2-oxoacetyl)-L-phenylalanyl- L-phenylalanine **6d**.