

Supplementary Material

Synthesis of diN-Substituted Glycyl-Phenylalanine Derivatives by Using Ugi Four Component Reaction and their Potential as Acetylcholinesterase Inhibitors

Luis Prent-Peñaloza ¹, Alexander F. de la Torre ², José L. Velázquez-Libera ³, Margarita Gutiérrez ¹ and Julio Caballero ^{3,*}

¹ Organic Synthesis Laboratory and Biological Activity (LSO-Act-Bio), Institute of Chemistry of Natural Resources, Universidad de Talca, Casilla 747, Talca 3460000, Chile; luisprent@gmail.com (L.P.-P.); mgutierrez@utalca.cl (M.G.)

² Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad de Concepción, Concepción 4030000, Chile; afndz1982@gmail.com

³ Centro de Bioinformática y Simulación Molecular (CBSM), Universidad de Talca, Casilla 747, Talca 3460000, Chile; josevlibera2010@gmail.com

* Correspondence: jcaballero@utalca.cl; Tel.: +56-712-418-850

Table of contents

Figure S1. FT-IR spectrum in KBr for 7a .	3
Figure S2. 400 MHz ¹ H-NMR spectrum in d ₆ -DMSO for 7a .	3
Figure S3. 400 MHz ¹³ C-NMR spectrum in d ₆ -DMSO for 7a .	4
Figure S4. 400 MHz APT spectrum in d ₆ -DMSO for 7a .	4
Figure S5. 400 MHz HSQC spectrum in d ₆ -DMSO for 7a .	5
Figure S6. 400 MHz HMBC spectrum in d ₆ -DMSO for 7a .	5
Figure S7. 400 MHz COSY spectrum in d ₆ -DMSO for 7a .	6
Figure S8. High-resolution mass spectrometry -ESI spectrum of 7a .	6
Figure S9. FT-IR spectrum in KBr for 7b .	7
Figure S10. 400 MHz ¹ H-NMR spectrum in d ₆ -DMSO for 7b .	7
Figure S11. 400 MHz ¹³ C-NMR spectrum in d ₆ -DMSO for 7b .	8
Figure S12. 400 MHz APT spectrum in d ₆ -DMSO for 7b .	8
Figure S13. 400 MHz HSQC spectrum in d ₆ -DMSO for 7b .	9
Figure S14. 400 MHz HMQC spectrum in d ₆ -DMSO for 7b .	9
Figure S15. 400 MHz COSY spectrum in d ₆ -DMSO for 7b .	9
Figure S16. High-resolution mass spectrometry -ESI spectrum of 7b .	10
Figure S17. FT-IR spectrum in KBr for 7c .	10
Figure S18. 400 MHz ¹ H-NMR spectrum in d ₆ -DMSO for 7c .	11
Figure S19. 400 MHz ¹³ C-NMR spectrum in d ₆ -DMSO for 7c .	11
Figure S20. 400 MHz APT spectrum in d ₆ -DMSO for 7c .	12
Figure S21. 400 MHz HSQC spectrum in d ₆ -DMSO for 7c .	12

Figure S22. 400 MHz HMBC spectrum in d ₆ -DMSO for 7c	12
Figure S23. 400 MHz COSY spectrum in d ₆ -DMSO for 7c	13
Figure S24. High-resolution mass spectrometry -ESI spectrum of 7c	13
Figure S25. FT-IR spectrum in KBr for 6d	14
Figure S26. 400 MHz ¹ H-NMR spectrum in d ₆ -DMSO for 6d	14
Figure S27. 400 MHz ¹³ C-NMR spectrum in d ₆ -DMSO for 6d	15
Figure S28. 400 MHz APT spectrum in d ₆ -DMSO for 6d	15
Figure S29. 400 MHz HSQC spectrum in d ₆ -DMSO for 6d	15
Figure S30. 400 MHz HMQC spectrum in d ₆ -DMSO for 6d	16
Figure S31. 400 MHz COSY spectrum in d ₆ -DMSO for 6d	16
Figure S32. High-resolution mass spectrometry -ESI spectrum of 6d	16
Figure S33. FT-IR spectrum in KBr for 6e	17
Figure S34. 400 MHz ¹ H-NMR spectrum in d ₆ -DMSO for 6e	17
Figure S35. 400 MHz ¹³ C-NMR spectrum in d ₆ -DMSO for 6e	18
Figure S36. 400 MHz APT spectrum in d ₆ -DMSO for 6e	18
Figure S37. 400 MHz, HSQC spectrum in d ₆ -DMSO for 6e	18
Figure S38. 400 MHz, HMQC spectrum in d ₆ -DMSO for 6e	19
Figure S39. 400 MHz, COSY spectrum in d ₆ -DMSO for 6e	19
Figure S40. High-resolution mass spectrometry -ESI spectrum of 6e	19

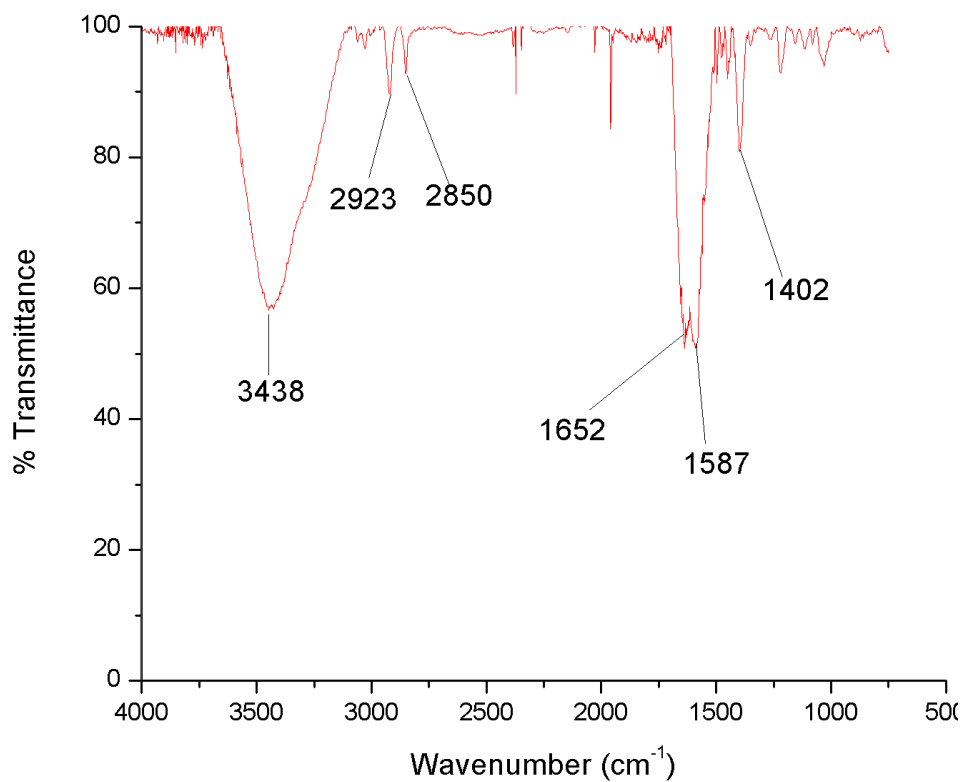


Figure S1. FT-IR spectrum in KBr for 7a.

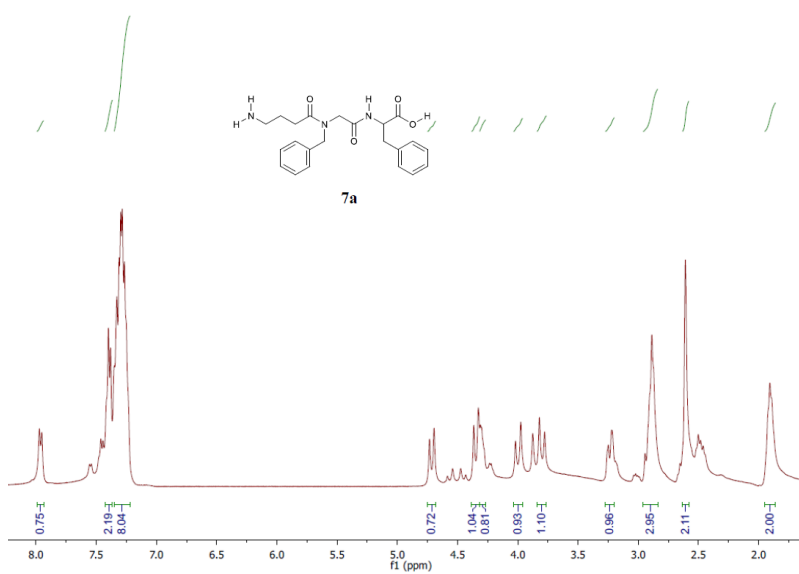


Figure S2. 400 MHz ¹H-NMR spectrum in d₆-DMSO for 7a.

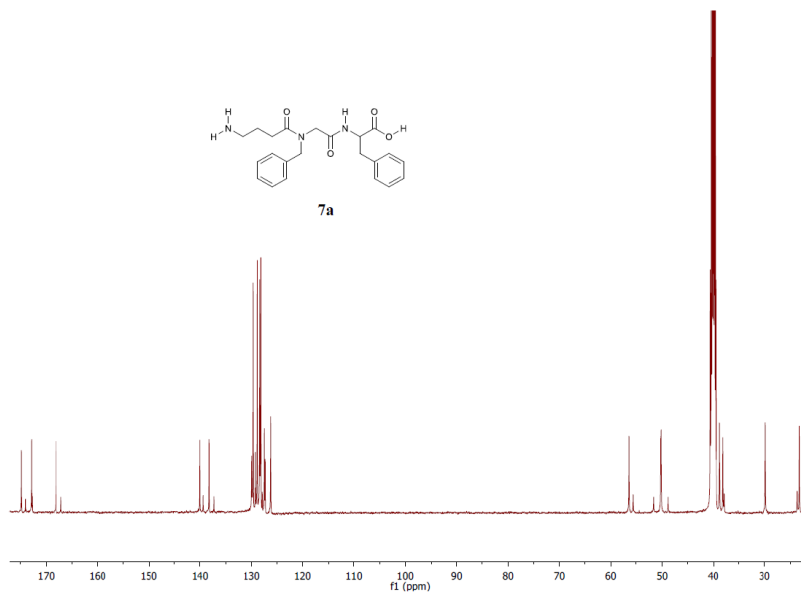


Figure S3. 400 MHz ^{13}C -NMR spectrum in d_6 -DMSO for **7a**.

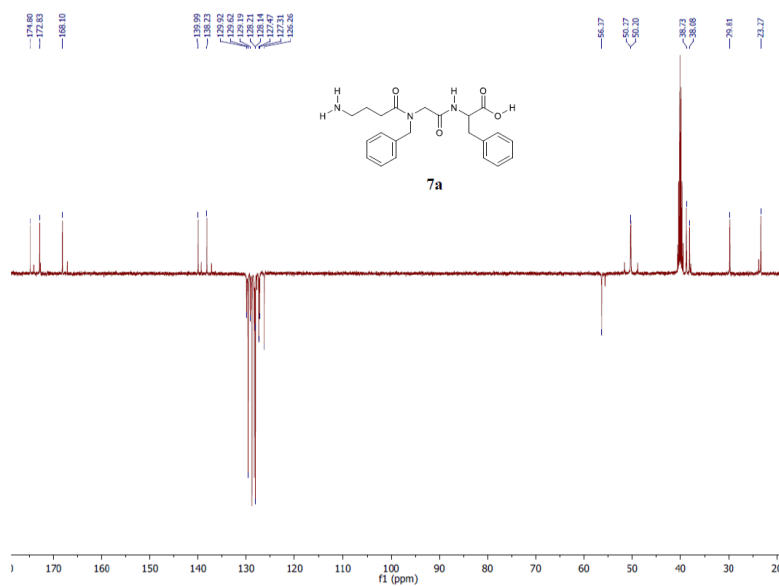


Figure S4. 400 MHz APT spectrum in d_6 -DMSO for **7a**.

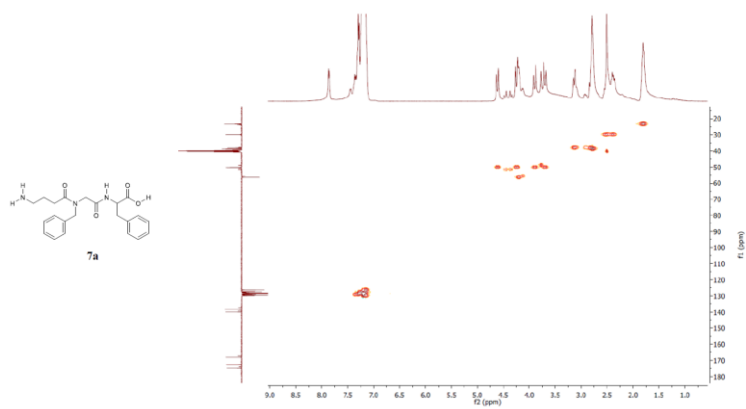


Figure S5. 400 MHz HSQC spectrum in d_6 -DMSO for **7a**.

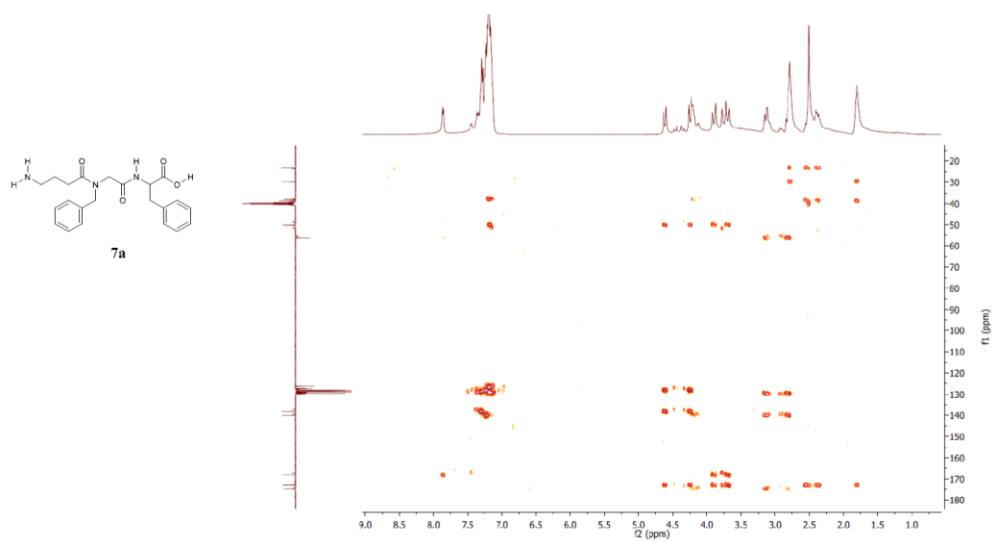


Figure S6. 400 MHz HMBC spectrum in d_6 -DMSO for **7a**.

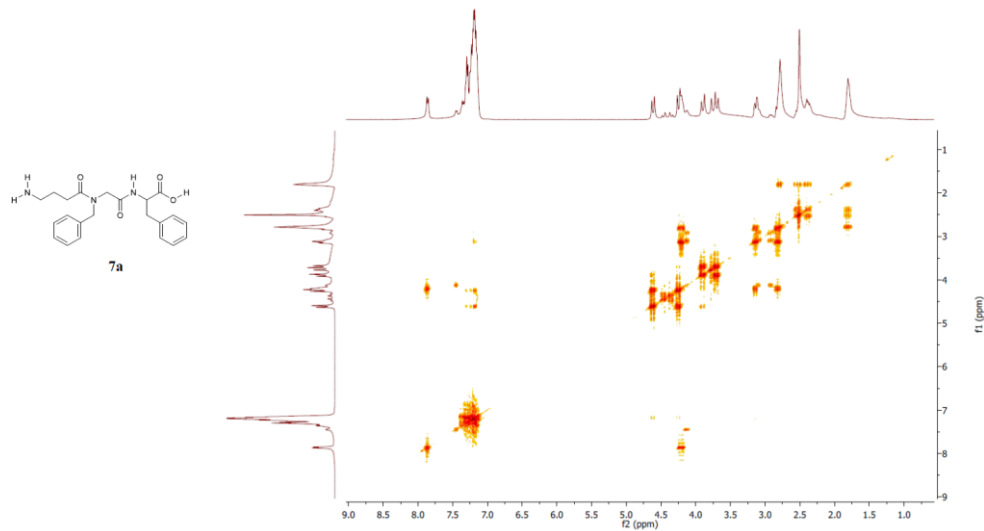


Figure S7. 400 MHz COSY spectrum in d_6 -DMSO for **7a**.

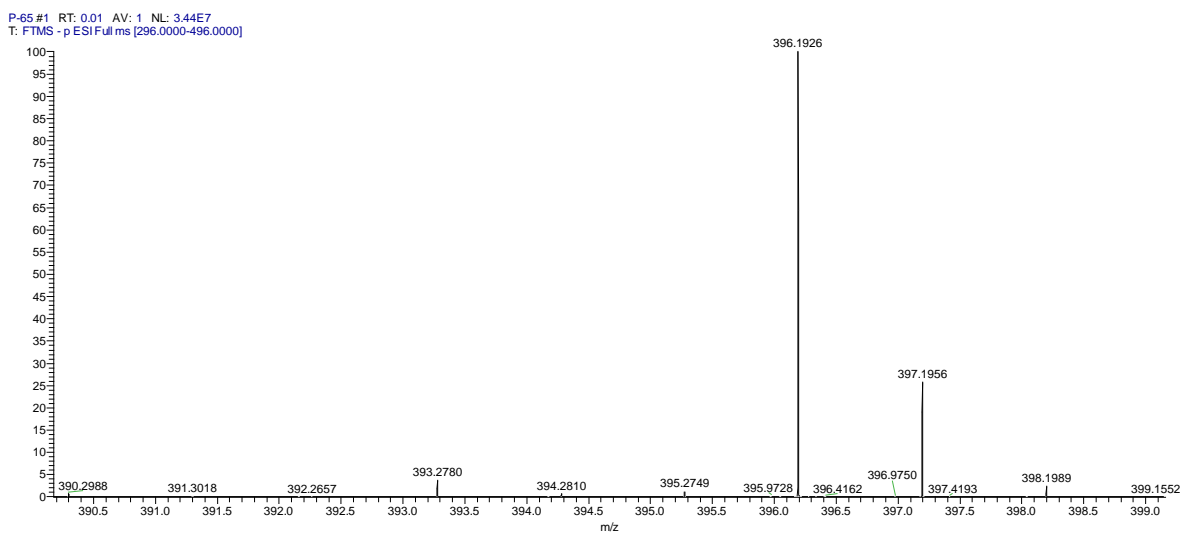


Figure S8. High-resolution mass spectrometry -ESI spectrum of **7a**.

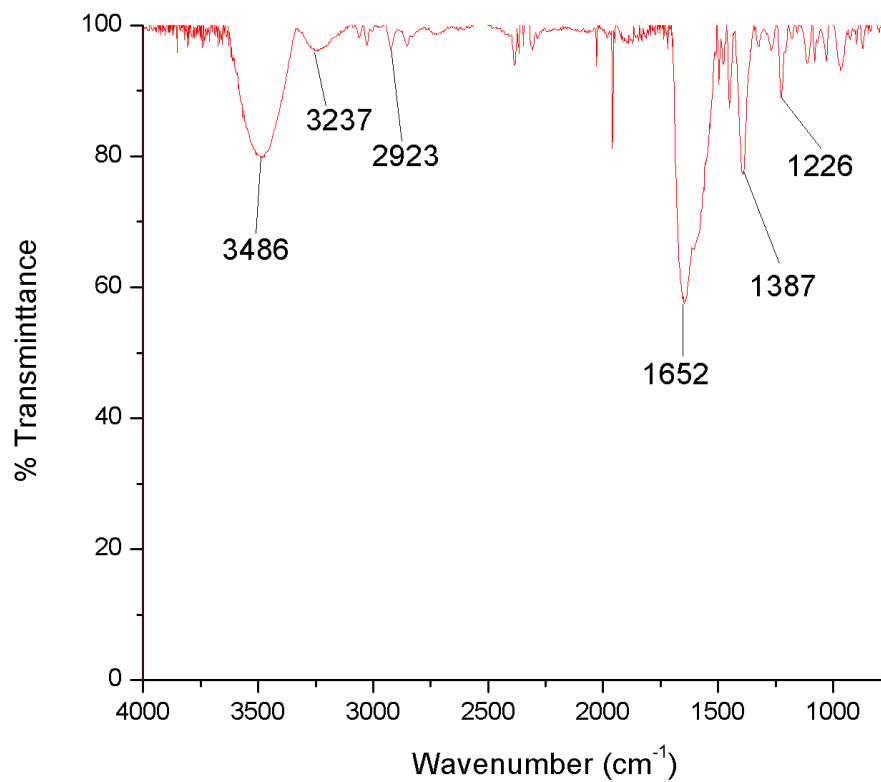


Figure S9. FT-IR spectrum in KBr for **7b**.

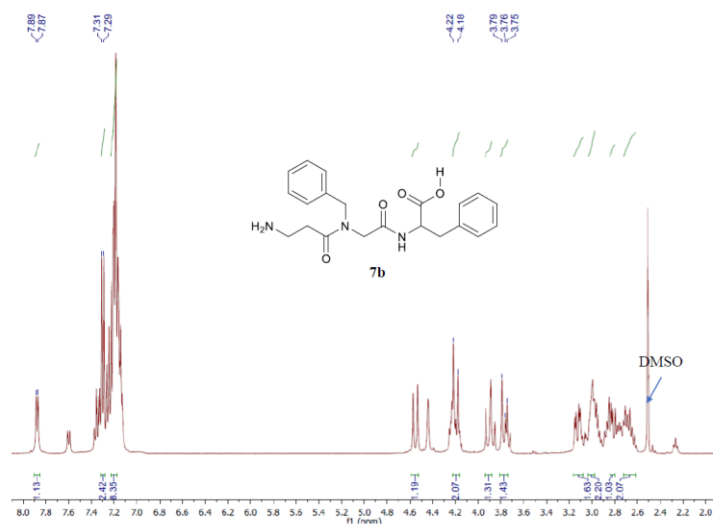


Figure S10. 400 MHz ¹H-NMR spectrum in d₆-DMSO for **7b**.

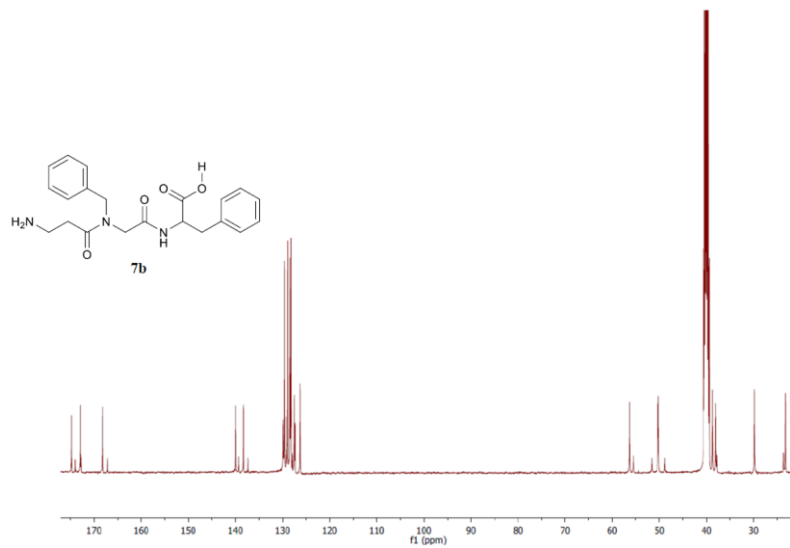


Figure S11. 400 MHz ^{13}C -NMR spectrum in d_6 -DMSO for **7b**.

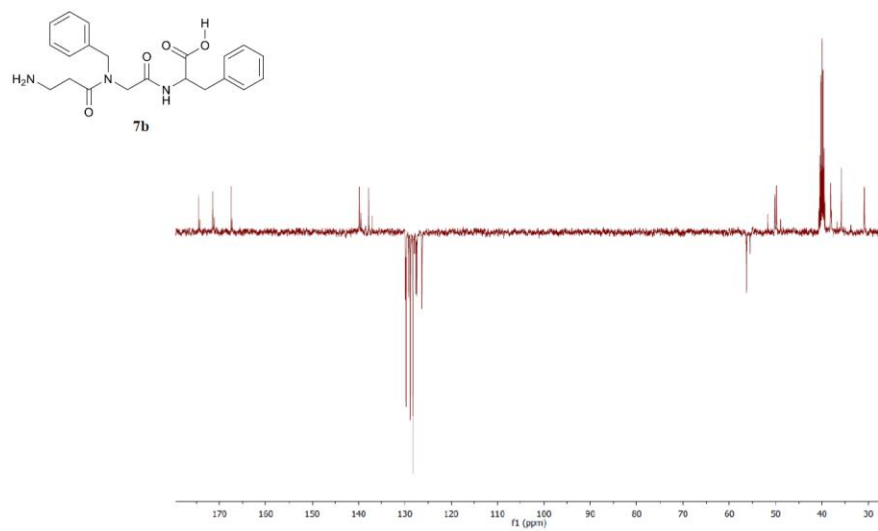


Figure S12. 400 MHz APT spectrum in d_6 -DMSO for **7b**.

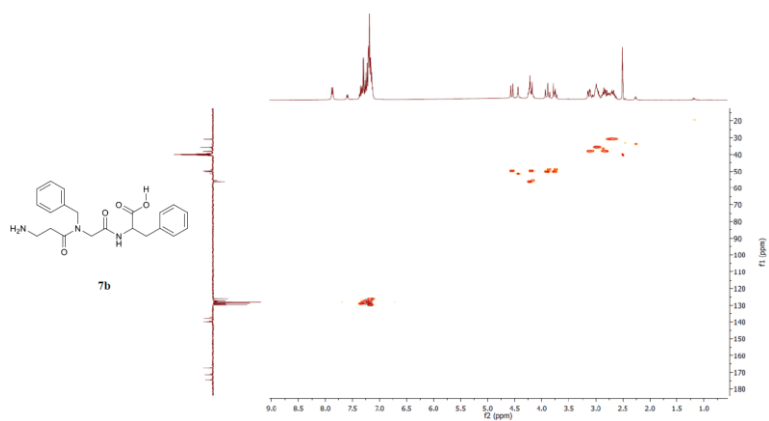


Figure S13. 400 MHz HSQC spectrum in d₆-DMSO for **7b**.

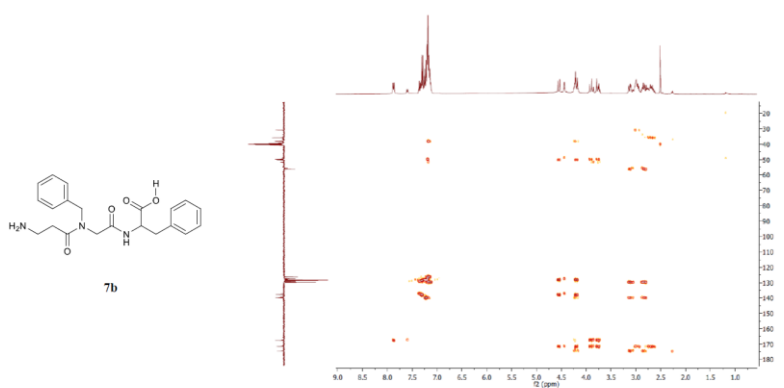


Figure S14. 400 MHz HMQC spectrum in d₆-DMSO for **7b**.

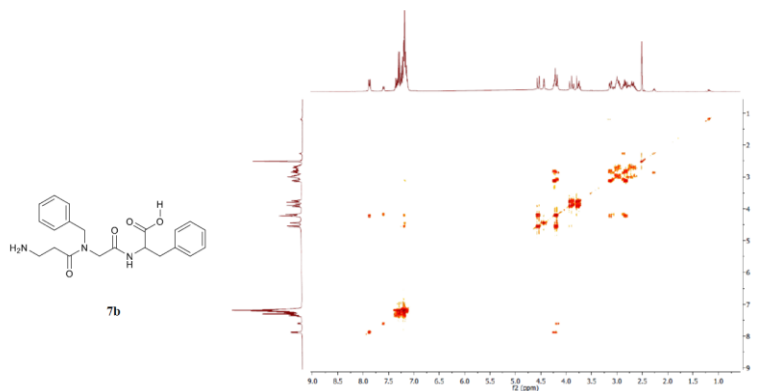


Figure S15. 400 MHz COSY spectrum in d₆-DMSO for **7b**.

P-68 #1 RT: 0.01 AV: 1 NL: 2.13E7
T: FTMS - p ESI Full ms [283.0000-483.0000]

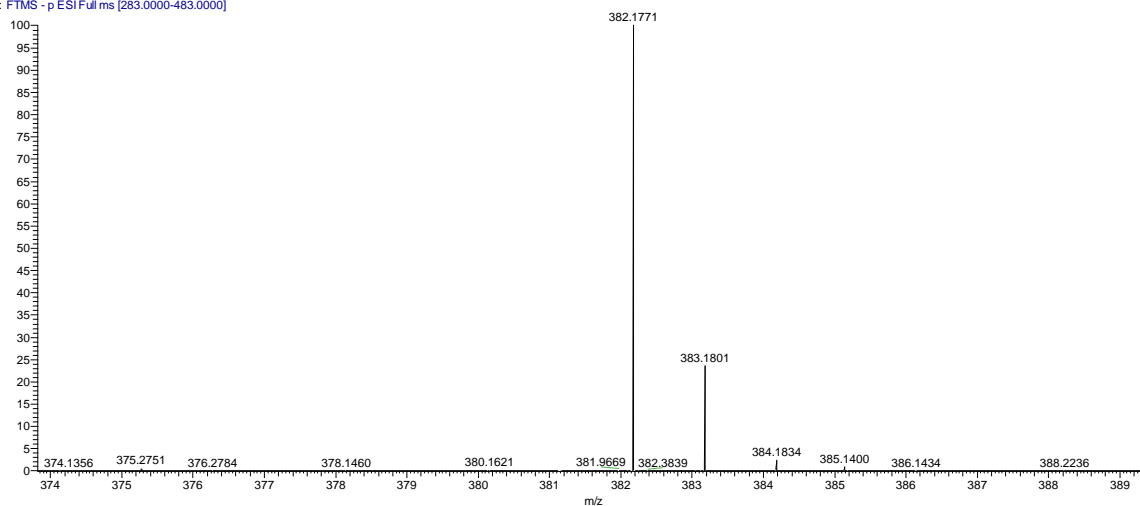


Figure S16. High-resolution mass spectrometry -ESI spectrum of 7b.

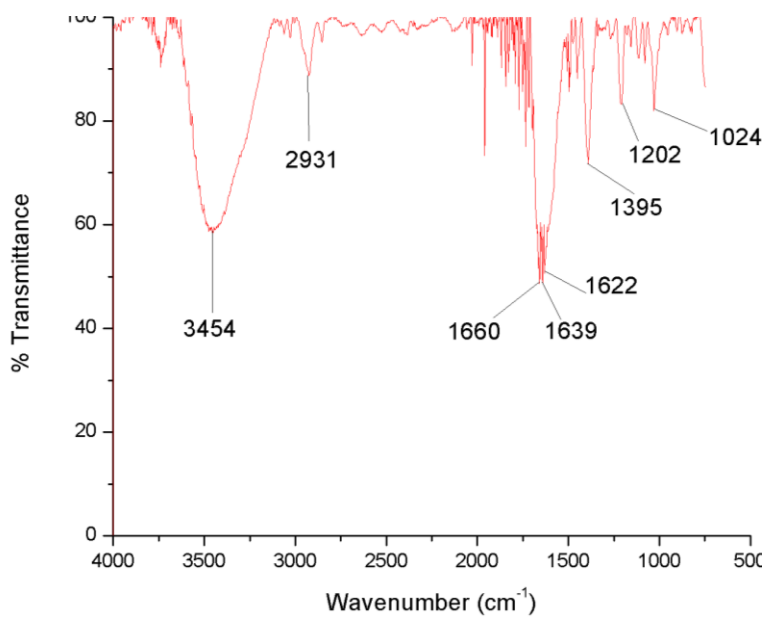


Figure S17. FT-IR spectrum in KBr for 7c.

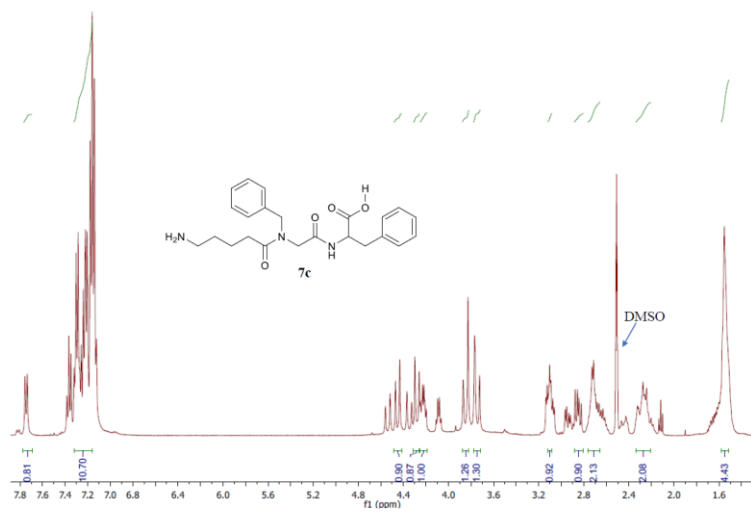


Figure S18. 400 MHz ^1H -NMR spectrum in d_6 -DMSO for 7c.

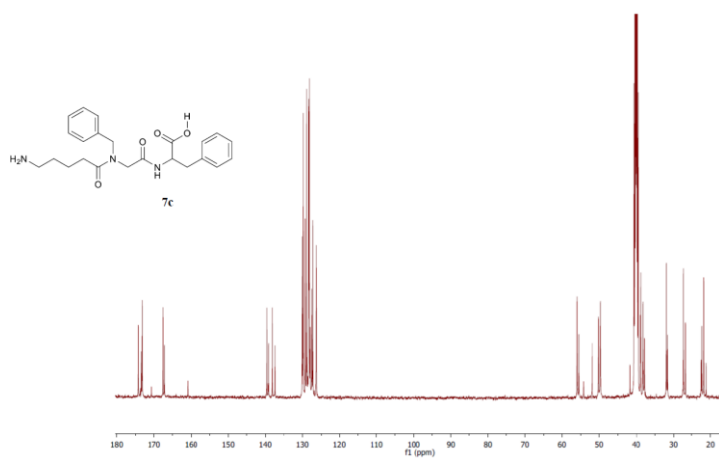
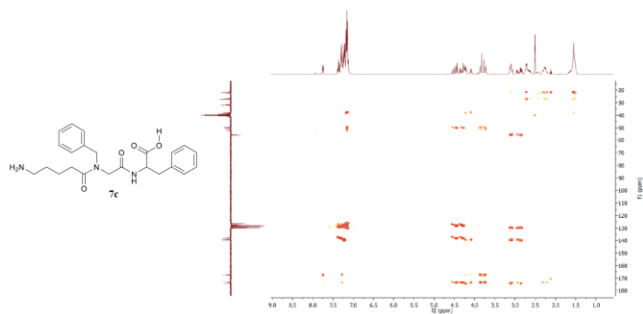
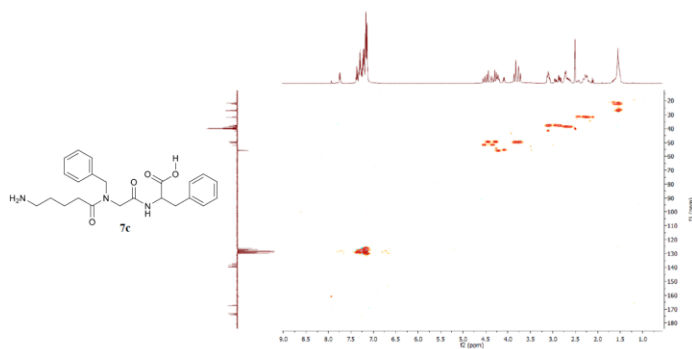
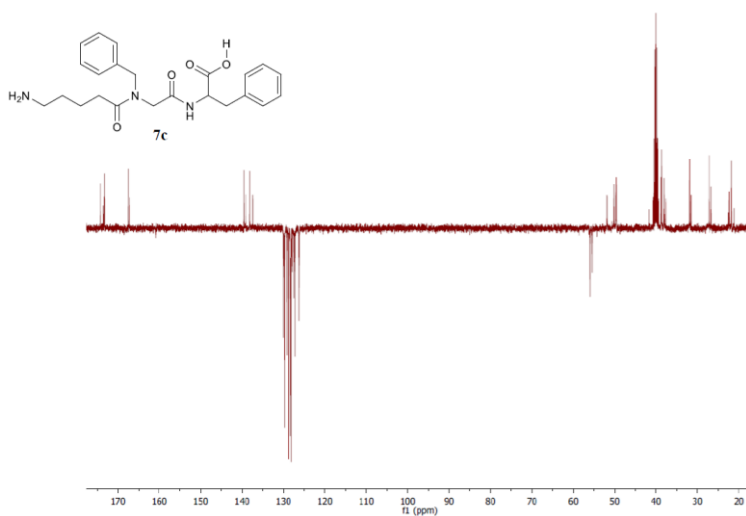


Figure S19. 400 MHz ^{13}C -NMR spectrum in d_6 -DMSO for 7c.



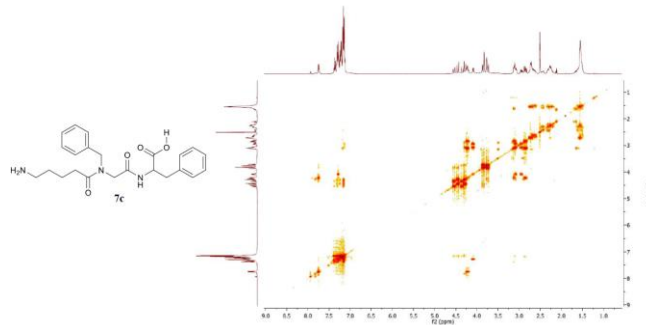


Figure S23. 400 MHz COSY spectrum in d_6 -DMSO for **7c**.

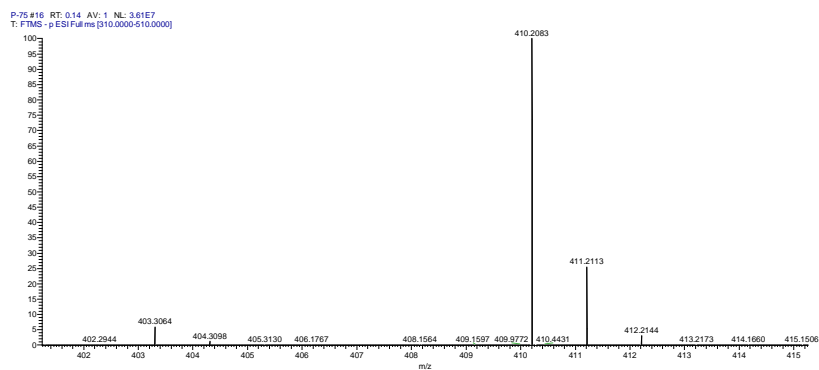


Figure S24. High-resolution mass spectrometry -ESI spectrum of **7c**.

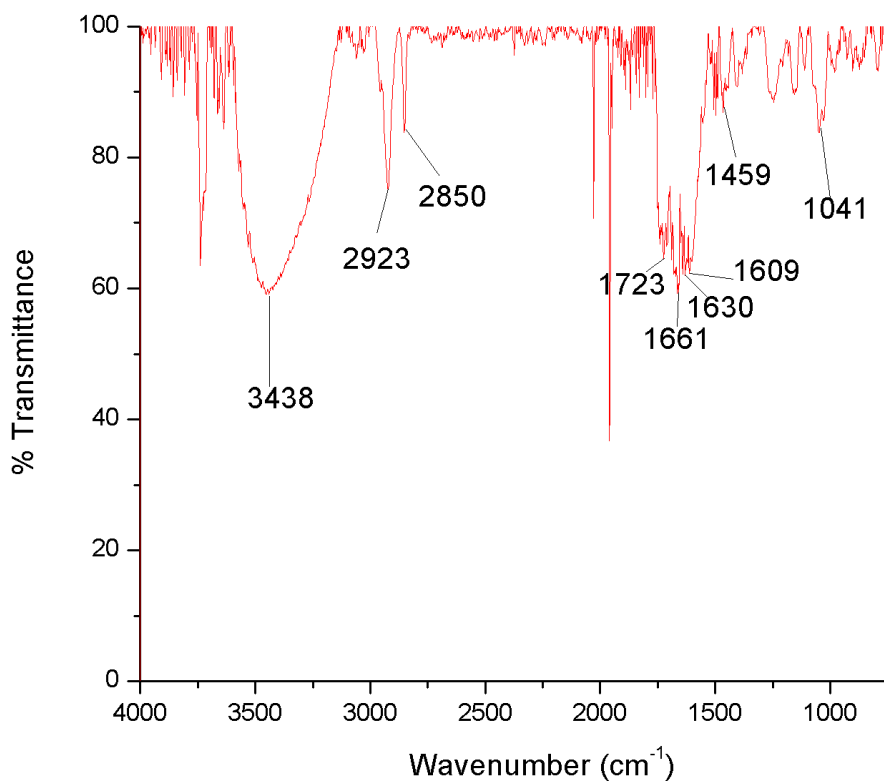


Figure S25. FT-IR spectrum in KBr for **6d**.

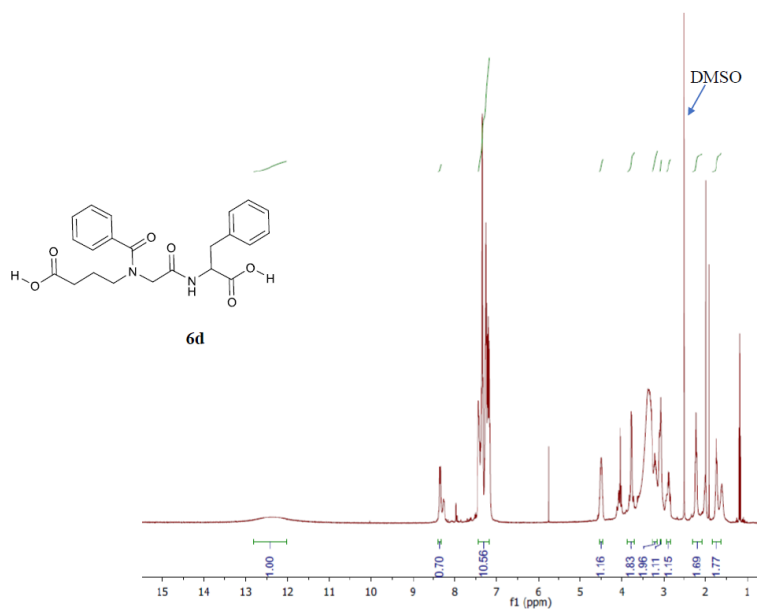


Figure S26. 400 MHz ^1H -NMR spectrum in d_6 -DMSO for **6d**.

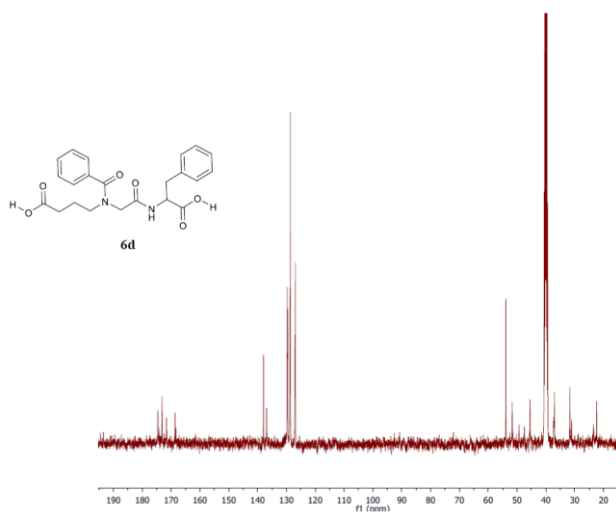
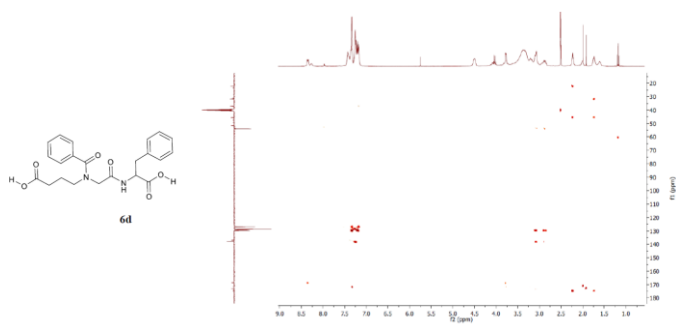
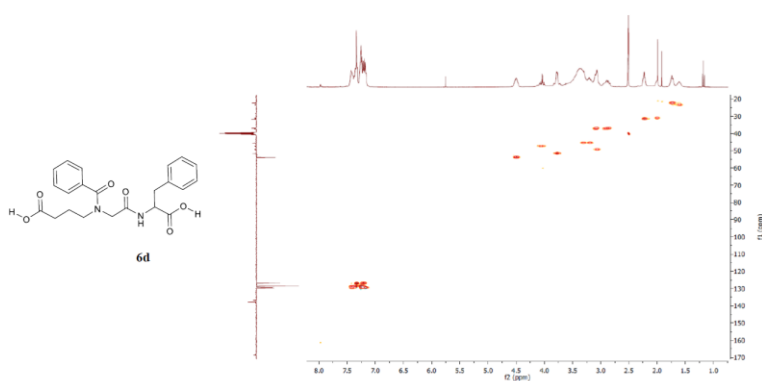
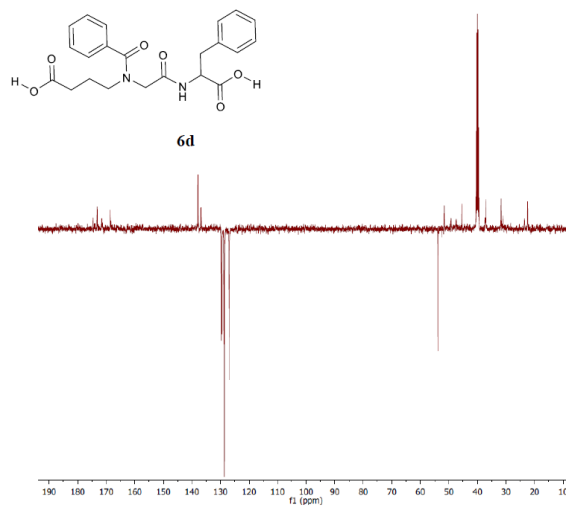


Figure S27. 400 MHz ^{13}C -NMR spectrum in d_6 -DMSO for **6d**.



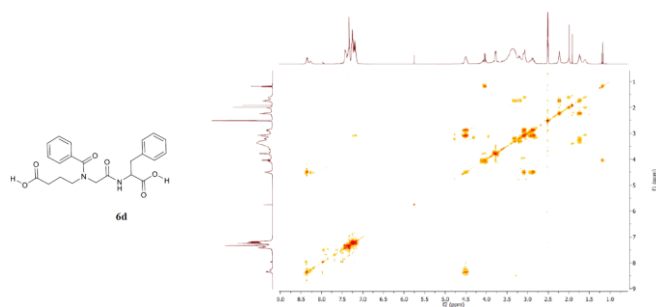


Figure S31. 400 MHz COSY spectrum in d_6 -DMSO for **6d**.

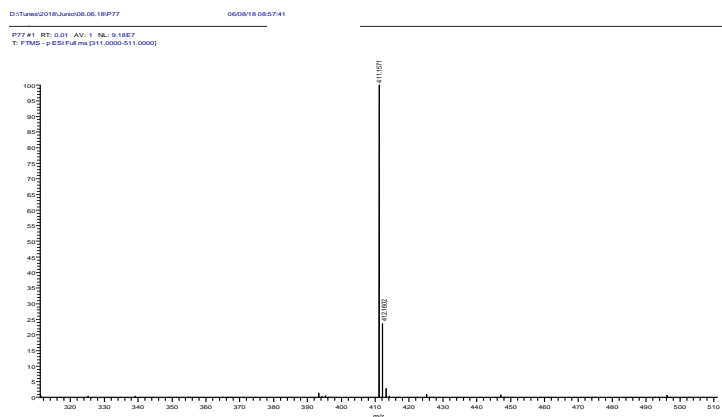


Figure S32. High-resolution mass spectrometry -ESI spectrum of **6d**.

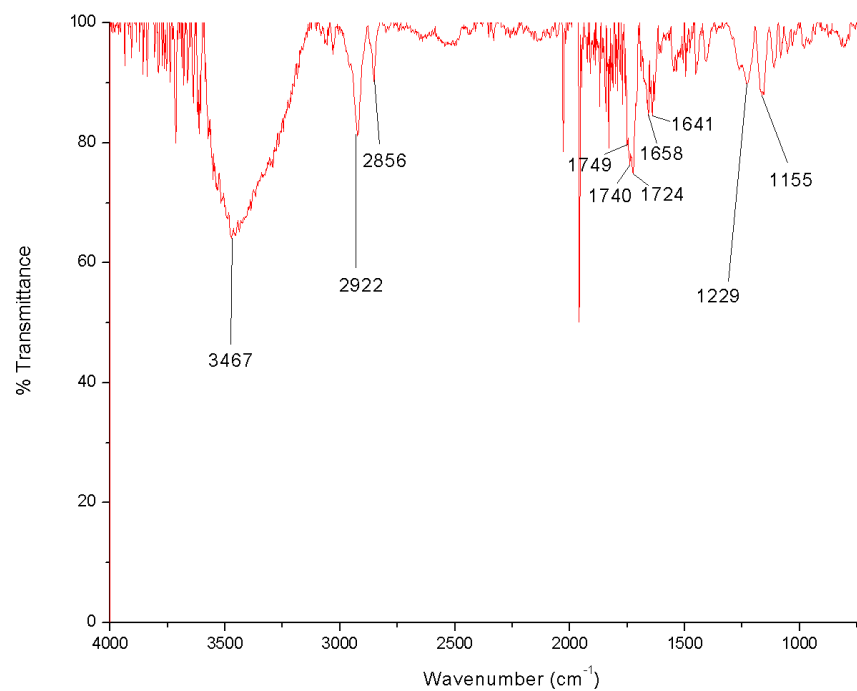


Figure S33. FT-IR spectrum in KBr for **6e**.

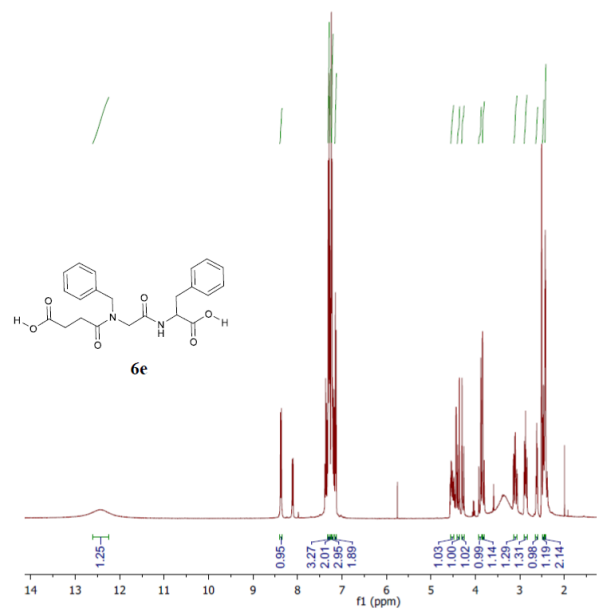


Figure S34. 400 MHz ¹H-NMR spectrum in d₆-DMSO for **6e**.

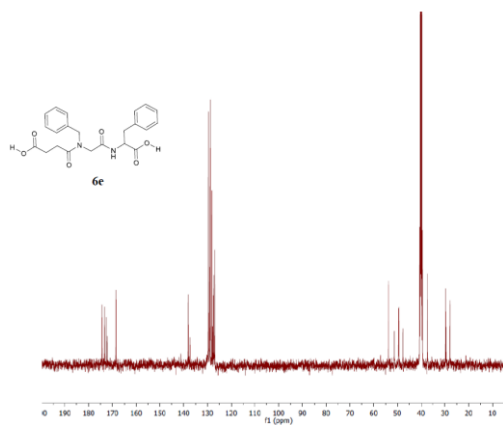


Figure S35. 400 MHz ^{13}C -NMR spectrum in d_6 -DMSO for **6e**.

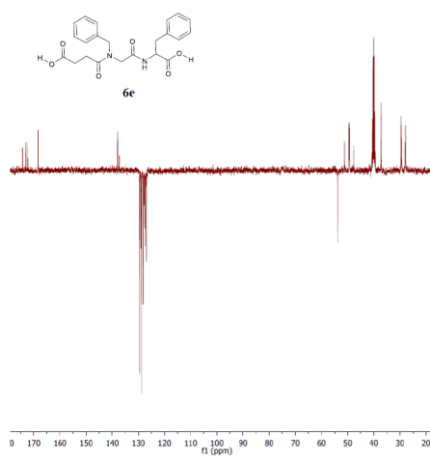


Figure S36. 400 MHz APT spectrum in d_6 -DMSO for **6e**.

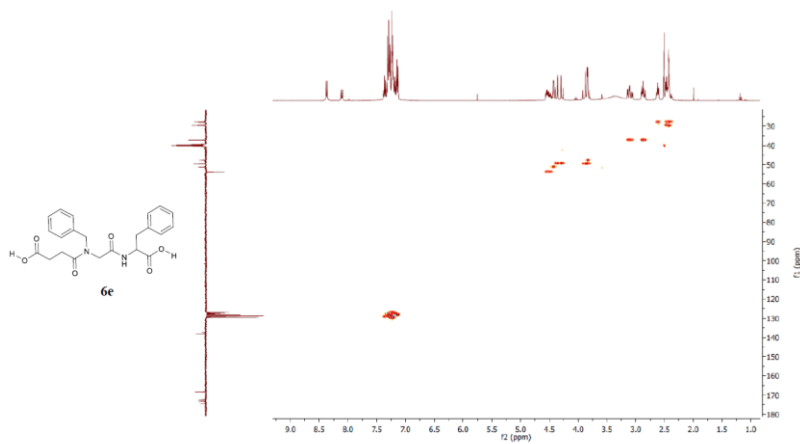


Figure S37. 400 MHz, HSQC spectrum in d_6 -DMSO for **6e**.

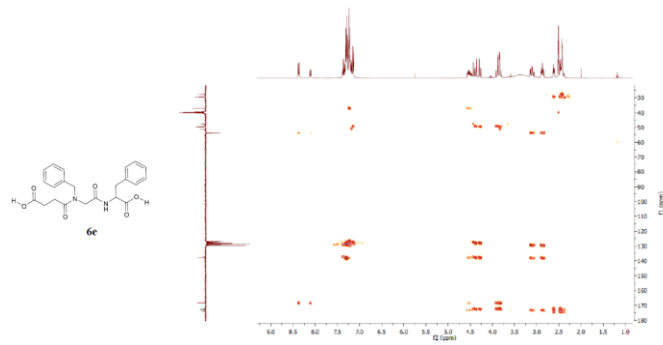


Figure S38. 400 MHz, HMQC spectrum in d_6 -DMSO for **6e**.

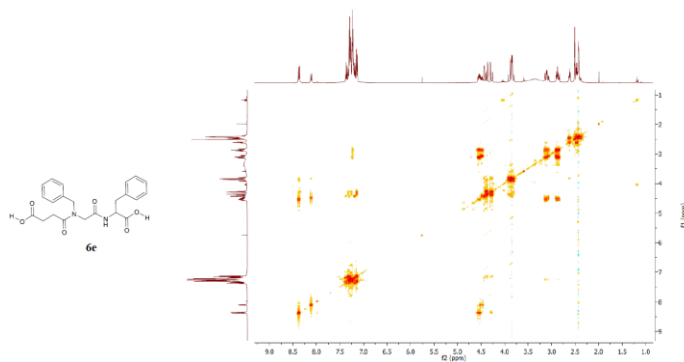


Figure S39. 400 MHz, COSY spectrum in d_6 -DMSO for **6e**.

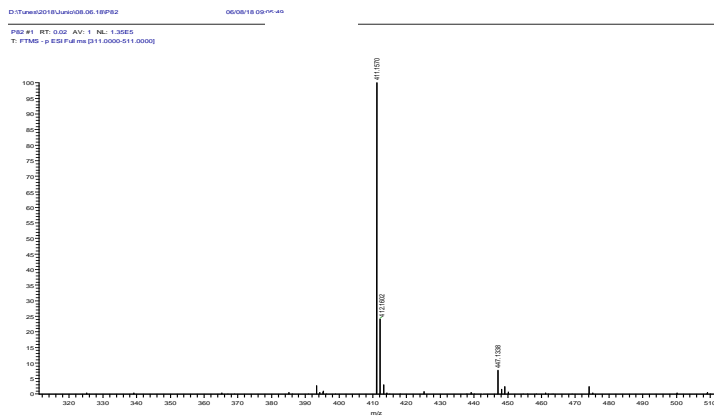


Figure S40. High-resolution mass spectrometry -ESI spectrum of **6e**.