Supplementary Materials

Preparation and Use of a General Solid-Phase Intermediate to Biomimetic Scaffolds and Peptide Condensations

J. Geno Samaritoni 1*, Jacek G. Martynow 2, Martin J. O’Donnell 1 and William L. Scott 1

1 Indiana University Purdue University Indianapolis, Department of Chemistry and Chemical Biology, 402 N. Blackford St., Indianapolis 46202, Indiana; modonnel@iupui.edu (M.J.O.); wscott@iupui.edu (W.L.S.)
2 Melinta Therapeutics, Inc., 300 George Street, S 301, New Haven, CT 06511; jmartynow@melinta.com
* Correspondence: jsamarit@iupui.edu; Tel.: +1-317-274-6872

Received: 23 June 2018; Accepted: 14 July 2018; Published: date

Table of Contents

Figure S1. Proton NMR Spectrum of 19a in CDCl3 ................................................................. 5
Figure S2. Carbon-13 NMR Spectrum of 19a in CDCl3 ......................................................... 6
Figure S3. Proton NMR Spectrum of 19b in CDCl3 ................................................................. 7
Figure S4. Carbon-13 NMR Spectrum of 19b in CDCl3 ......................................................... 8
Figure S5. Proton NMR Spectrum of 19c in CDCl3 ................................................................. 9
Figure S6. Carbon-13 NMR Spectrum of 19c in CDCl3 ......................................................... 10
Figure S7. Proton NMR Spectrum of α-21c and β-21c in CDCl3 .............................................. 11
Figure S8. Carbon-13 NMR Spectrum of α-21c and β-21c in CDCl3 ....................................... 12
Figure S9. Proton NMR Spectrum of 24c (earlier R1) in CD3OD ........................................... 13
Figure S10. Carbon-13 NMR Spectrum of 24c (earlier R1) in CD3OD ...................................... 14
Figure S11. Proton NMR Spectrum of 24c (later R1) in CDCl3 ................................................. 15
Figure S12. Carbon-13 NMR Spectrum of 24c (later R1) in CDCl3 ........................................... 16
Figure S13. Proton NMR Spectrum of β-26c in CD2OD .......................................................... 17
Figure S14. Carbon-13 NMR Spectrum of β-26c in CD3OD .................................................. 18
Figure S15. Proton NMR Spectrum of 31 in CDCl3 ................................................................. 19
Figure S16. Carbon-13 NMR Spectrum of 31 in CDCl$_3$ ................................................................. 20
Figure S17. Proton NMR Spectrum of $\alpha$-33a in CDCl$_3$ .............................................................. 21
Figure S18. Carbon-13 NMR Spectrum of $\alpha$-33a in CDCl$_3$ .......................................................... 22
Figure S19. Proton NMR Spectrum of $\beta$-33a in CDCl$_3$ ................................................................. 23
Figure S20. Carbon-13 NMR Spectrum of $\beta$-33a in CDCl$_3$ ........................................................... 24
Figure S21. Proton NMR Spectrum of $\beta$-33b in CDCl$_3$ ................................................................. 25
Figure S22. Carbon-13 NMR Spectrum of $\beta$-33b in CDCl$_3$ ........................................................... 26
Figure S23. Proton NMR Spectrum of $\alpha$-33b in CDCl$_3$ ................................................................. 27
Figure S24. Carbon-13 NMR Spectrum of $\alpha$-33b in CDCl$_3$ ........................................................... 28
Figure S25. Proton NMR Spectrum of $\beta$-33c in CDCl$_3$ ................................................................. 29
Figure S26. Carbon-13 NMR Spectrum of $\beta$-33c in CDCl$_3$ ........................................................... 30
Figure S27. Proton NMR Spectrum of $\alpha$-33c in CDCl$_3$ ................................................................. 31
Figure S28. Carbon-13 NMR Spectrum of $\alpha$-33c in CDCl$_3$ ........................................................... 32
Figure S29. Proton NMR Spectrum of $\beta$-34a in CDCl$_3$ ................................................................. 33
Figure S30. Carbon-13 NMR Spectrum of $\beta$-34a in CDCl$_3$ ........................................................... 34
Figure S31. Proton NMR Spectrum of $\alpha$-34a in CDCl$_3$ ................................................................. 35
Figure S32. Carbon-13 NMR Spectrum of $\alpha$-34a in CDCl$_3$ ........................................................... 36
Figure S33. Proton NMR Spectrum of $\alpha$-35a in CDCl$_3$ ................................................................. 37
Figure S34. Carbon-13 NMR Spectrum of $\alpha$-35a in CDCl$_3$ ........................................................... 38
Figure S35. Proton NMR Spectrum of $\beta$-35a in CDCl$_3$ ................................................................. 39
Figure S36. Carbon-13 NMR Spectrum of $\beta$-35a in CDCl$_3$ ........................................................... 40
Figure S37. Proton NMR Spectrum of $\beta$-35b in CDCl$_3$ ................................................................. 41
Figure S38. Carbon-13 NMR Spectrum of $\beta$-35b in CDCl$_3$ ........................................................... 42
Figure S39. Proton NMR Spectrum of $\alpha$-35b in CDCl$_3$ ................................................................. 43
Figure S40. Carbon-13 NMR Spectrum of $\alpha$-35b in CDCl$_3$ ........................................................... 44
Figure S41. Proton NMR Spectrum of $\beta$-35c in CDCl$_3$ ................................................................. 45
Figure S42. Carbon-13 NMR Spectrum of $\beta$-35c in CDCl$_3$ ........................................................... 46
Figure S43. Proton NMR Spectrum of $\alpha$-35c in CDCl$_3$ ................................................................. 47
Figure S44. Carbon-13 NMR Spectrum of $\alpha$-35c in CDCl$_3$ ........................................................... 48
Figure S45. Proton NMR Spectrum of $\beta$-36a in CDCl$_3$ ................................................................. 49
Figure S46. Carbon-13 NMR Spectrum of $\beta$-36a in CDCl$_3$ ........................................................... 50
Figure S47. Proton NMR Spectrum of $\alpha$-36a in CDCl$_3$ ................................................................. 51
Figure S48. Carbon-13 NMR Spectrum of $\alpha$-36a in CDCl$_3$ ................................................................. 52
Figure S49. Proton NMR Spectrum of $\beta$-36b in CDCl$_3$ ........................................................................ 53
Figure S50. Carbon-13 NMR Spectrum of $\beta$-36b in CDCl$_3$ ................................................................. 54
Figure S51. Proton NMR Spectrum of $\alpha$-36b in CDCl$_3$ ........................................................................ 55
Figure S52. Carbon-13 NMR Spectrum of $\beta$-36b in CDCl$_3$ ................................................................. 56
Figure S53. Proton NMR Spectrum of $\alpha$-36b in CDCl$_3$ ........................................................................ 57
Figure S54. Carbon-13 NMR Spectrum of $\beta$-36c in CDCl$_3$ ................................................................. 58
Figure S55. Proton NMR Spectrum of $\alpha$-36c in CDCl$_3$ ........................................................................ 59
Figure S56. Carbon-13 NMR Spectrum of $\beta$-36c in CDCl$_3$ ................................................................. 60
Figure S57. Proton NMR Spectrum of $\alpha$-30b in CDCl$_3$ ........................................................................ 61
Figure S58. Carbon-13 NMR Spectrum of $\alpha$-30b in CDCl$_3$ ........................................................................ 62
Figure S59. Proton NMR Spectrum of $\beta$-30b in CDCl$_3$ ........................................................................ 63
Figure S60. Carbon-13 NMR Spectrum of $\beta$-30b in CDCl$_3$ ........................................................................ 64
Figure S61. Proton NMR Spectrum of $\beta$-30c in CDCl$_3$ ........................................................................ 65
Figure S62. Carbon-13 NMR Spectrum of $\beta$-30c in CDCl$_3$ ........................................................................ 66
Figure S63. Proton NMR Spectrum of $\alpha$-30c in CDCl$_3$ ........................................................................ 67
Figure S64. Carbon-13 NMR Spectrum of $\alpha$-30c in CDCl$_3$ ........................................................................ 68
Figure S65. Proton NMR Spectrum of $\alpha$-37b in CDCl$_3$ ........................................................................ 69
Figure S66. Carbon-13 NMR Spectrum of $\alpha$-37b in CDCl$_3$ ........................................................................ 70
Figure S67. Proton NMR Spectrum of $\beta$-37b in CDCl$_3$ ........................................................................ 71
Figure S68. Carbon-13 NMR Spectrum of $\beta$-37b in CDCl$_3$ ........................................................................ 72
Figure S69. Proton NMR Spectrum of (Fmoc-Ala)$_2$O in CDCl$_3$ with Diisopropylurea (DIU) .................... 73
Figure S70. Proton NMR Spectrum of Boc-Cys(Trt)-Leu-OMe in CDCl$_3$ ...................................................... 74
Figure S71. Carbon-13 NMR Spectrum of Boc-Cys(Trt)-Leu-OMe in CDCl$_3$ ...................................................... 75
Figure S1. Proton NMR Spectrum of 19a in CDCl₃
Figure S2. Carbon-13 NMR Spectrum of 19a in CDCl₃
Figure S3. Proton NMR Spectrum of 19b in CDCl₃
Figure S4. Carbon-13 NMR Spectrum of 19b in CDCl₃
Figure S5. Proton NMR Spectrum of 19c in CDCl₃
Figure S6. Carbon-13 NMR Spectrum of 19c in CDCl₃
Figure S7. Proton NMR Spectrum of α-21c and β-21c in CDCl₃
Figure S8. Carbon-13 NMR Spectrum of α-21c and β-21c in CDCl₃
Figure S9. Proton NMR Spectrum of 24c (earlier R1) in CD$_3$OD
Figure S10. Carbon-13 NMR Spectrum of 24c (earlier R₃) in CD₃OD
Figure S11. Proton NMR Spectrum of 24c (later R) in CDCl₃
Figure S12. Carbon-13 NMR Spectrum of 24c (later R) in CDCl₃
Figure S13. Proton NMR Spectrum of $\beta$-26c in CD$_3$OD
Figure S14. Carbon-13 NMR Spectrum of β-26c in CD$_3$OD
Figure S15. Proton NMR Spectrum of 31 in CDCl₃
Figure S16. Carbon-13 NMR Spectrum of 31 in CDCl$_3$
Figure S17. Proton NMR Spectrum of α-33a in CDCl₃
Figure S18. Carbon-13 NMR Spectrum of α-33a in CDCl₃
Figure S19. Proton NMR Spectrum of β-33a in CDCl₃
Figure S20. Carbon-13 NMR Spectrum of β-33a in CDCl₃
Figure S21. Proton NMR Spectrum of β-33b in CDCl₃
Figure S22. Carbon-13 NMR Spectrum of $\beta$-33b in CDCl$_3$
Figure S23. Proton NMR Spectrum of α-33b in CDCl₃
Figure S24. Carbon-13 NMR Spectrum of $\alpha$-33b in CDCl$_3$
Figure S25. Proton NMR Spectrum of $\beta$-33c in CDCl$_3$
Figure S26. Carbon-13 NMR Spectrum of β-33c in CDCl₃
Figure S27. Proton NMR Spectrum of $\alpha$-33c in CDCl$_3$
Figure S28. Carbon-13 NMR Spectrum of α-33c in CDCl₃
Figure S29. Proton NMR Spectrum of β-34a in CDCl₃
Figure S30. Carbon-13 NMR Spectrum of β-34a in CDCl₃
Figure S31. Proton NMR Spectrum of $\alpha$-34a in CDCl$_3$
Figure S32. Carbon-13 NMR Spectrum of α-34a in CDCl₃
Figure S33. Proton NMR Spectrum of $\alpha$-35a in CDCl$_3$
Figure S34. Carbon-13 NMR Spectrum of \( \alpha \)-35a in CDCl\(_3\)
Figure S35. Proton NMR Spectrum of β-35a in CDCl₃
Figure S36. Carbon-13 NMR Spectrum of β-35a in CDCl$_3$
Figure S37. Proton NMR Spectrum of $\beta$-35b in CDCl$_3$
Figure S38. Carbon-13 NMR Spectrum of β-35b in CDCl₃
Figure S39. Proton NMR Spectrum of α-35b in CDCl₃
Figure S40. Carbon-13 NMR Spectrum of α-35b in CDCl₃
Figure S41. Proton NMR Spectrum of β-35c in CDCl₃
Figure S42. Carbon-13 NMR Spectrum of β-35c in CDCl₃
Figure S43. Proton NMR Spectrum of α-35c in CDCl$_3$
Figure S44. Carbon-13 NMR Spectrum of α-35c in CDCl₃
Figure S45. Proton NMR Spectrum of β-36a in CDCl₃
Figure S46. Carbon-13 NMR Spectrum of β-36a in CDCl₃
Figure S47. Proton NMR Spectrum of α-36a in CDCl₃
Figure S48. Carbon-13 NMR Spectrum of α-36a in CDCl₃
Figure S49. Proton NMR Spectrum of \( \beta-36b \) in CDCl\(_3\)
Figure S50. Carbon-13 NMR Spectrum of \( \beta-36b \) in CDCl\(_3\)
Figure S51. Proton NMR Spectrum of α-36b in CDCl₃
Figure S52. Carbon-13 NMR Spectrum of α-36b in CDCl$_3$
Figure S53. Proton NMR Spectrum of \( \alpha \)-36c in CDCl\(_3\)
Figure S54. Carbon-13 NMR Spectrum of α-36c in CDCl₃
Figure S55. Proton NMR Spectrum of β-36c in CDCl₃
Figure S56. Carbon-13 NMR Spectrum of \( \beta-36c \) in CDCl\(_3\)
Figure S57. Proton NMR Spectrum of α-30b in CDCl₃
Figure S58. Carbon-13 NMR Spectrum of α-30b in CDCl₃
Figure S59. Proton NMR Spectrum of β-30b in CDCl₃
Figure S60. Carbon-13 NMR Spectrum of β-30b in CDCl₃
Figure S61. Proton NMR Spectrum of β-30c in CDCl₃
Figure S62. Carbon-13 NMR Spectrum of β-30c in CDCl₃
Figure S63. Proton NMR Spectrum of $\alpha$-30c in CDCl$_3$
Figure S64. Carbon-13 NMR Spectrum of $\alpha$-30c in CDCl$_3$
Figure S65. Proton NMR Spectrum of \( \alpha\text{-37b} \) in CDCl\(_3\)
Figure S66. Carbon-13 NMR Spectrum of α-37b in CDCl₃
Figure S67. Proton NMR Spectrum of $\beta$-37b in CDCl$_3$
Figure S68. Carbon-13 NMR Spectrum of β-37b in CDCl₃
Figure S69. Proton NMR Spectrum of (Fmoc-Ala)$_2$O in CDCl$_3$ with Diisopropylurea (DIU)
Figure S70. Proton NMR Spectrum of Boc-Cys(Trt)-Leu-OMe in CDCl$_3$
Figure S71. Carbon-13 NMR Spectrum of Boc-Cys(Trt)-Leu-OMe in CDCl₃