

Supporting Information
for
The First Chalcone Derivatives of Valine-Based Spiro-cyclotriphosphazenes: In vitro Cytotoxic Properties, Molecular Docking and DNA Damage Mechanism Studies

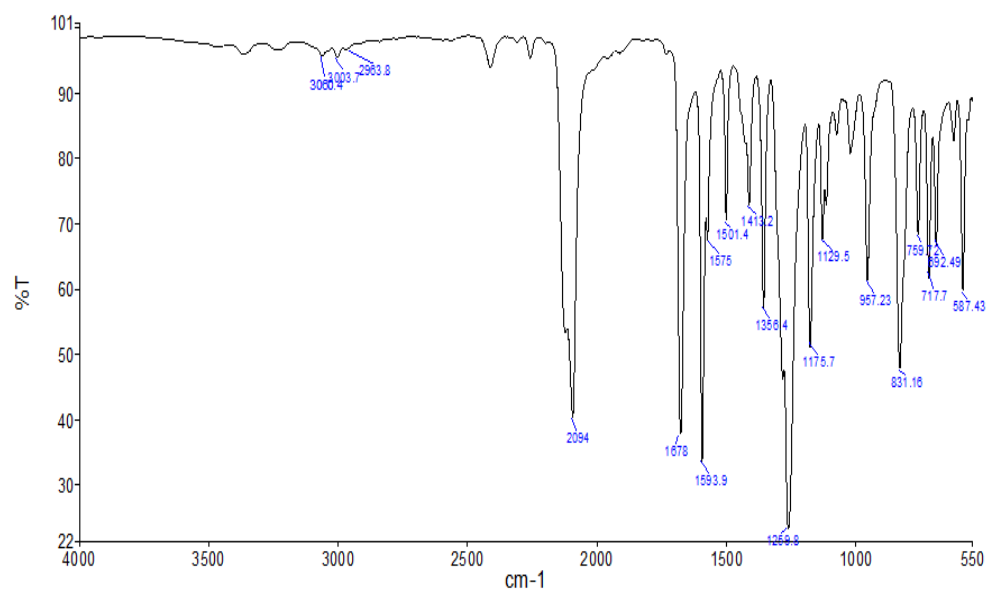


Figure S1. FT-IR (ATR) spectra of N_3 -AF

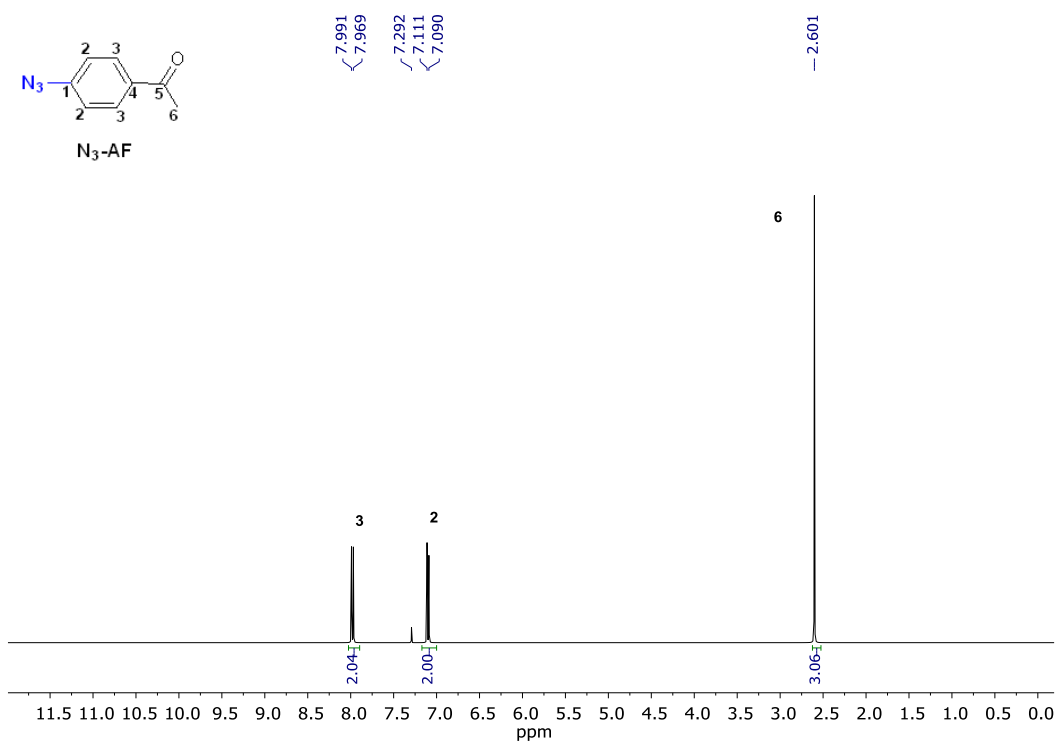


Figure S2. ^1H -NMR spectra of N_3 -AF (DMSO-d_6)

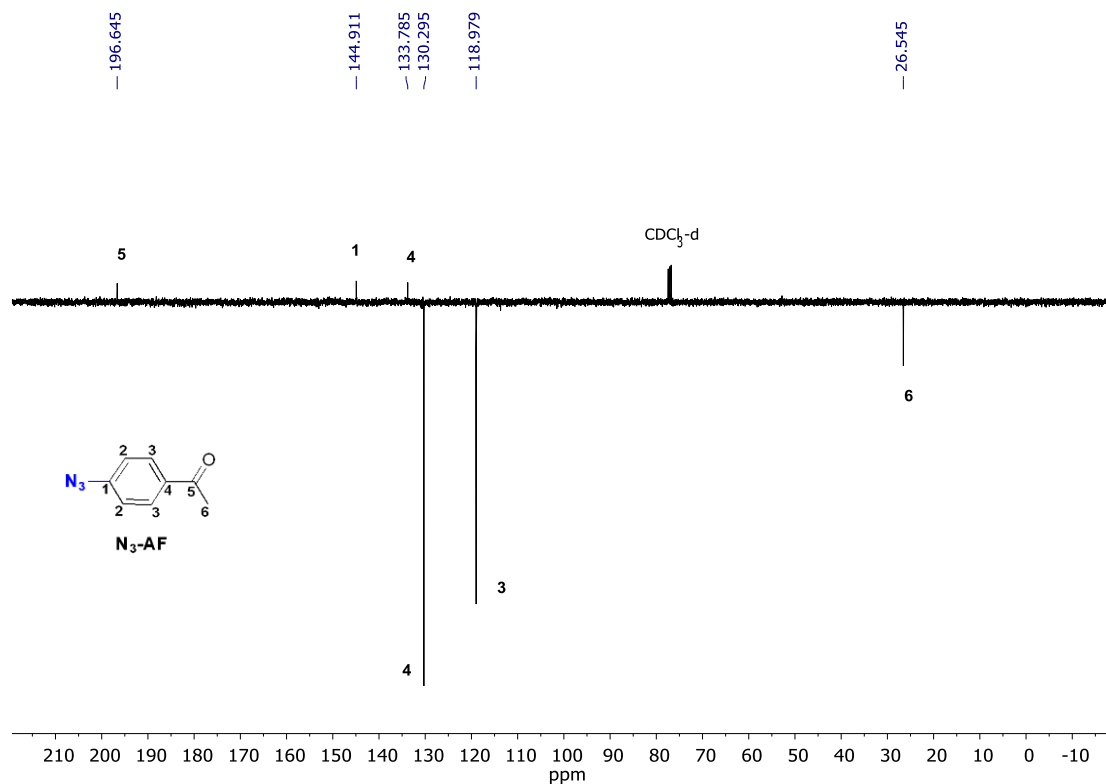


Figure S3. ¹³C-NMR spectra of N₃-AF (DMSO-d₆)

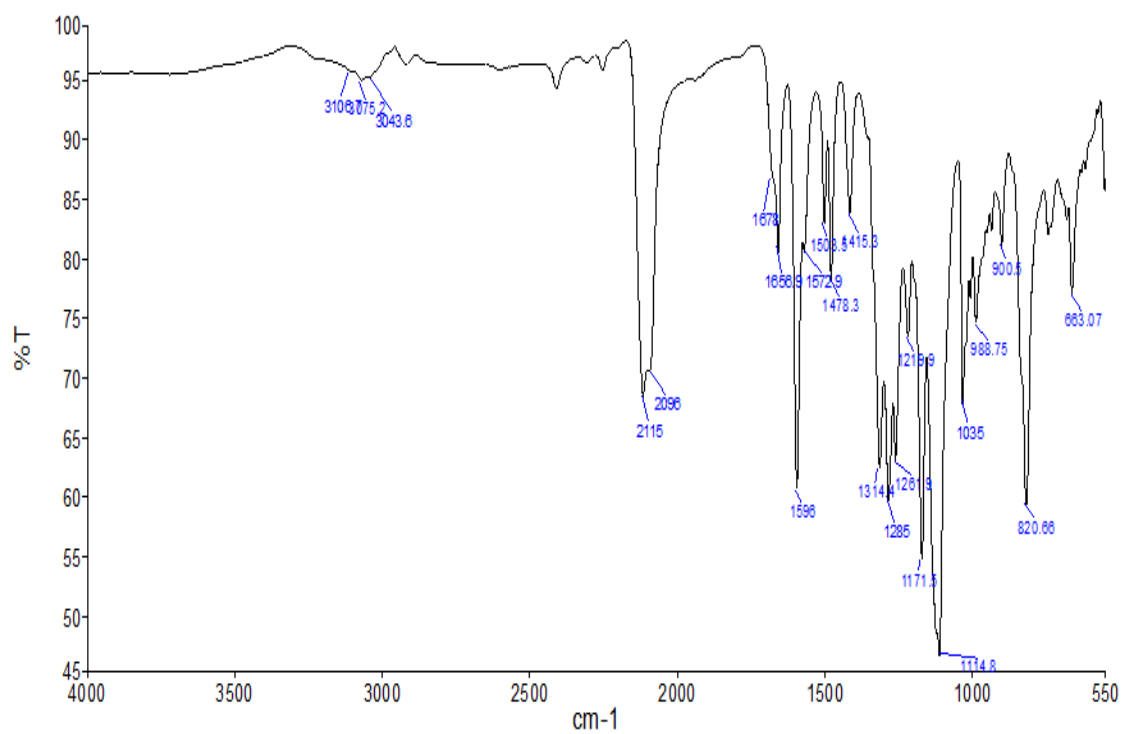


Figure S4. FT-IR (ATR) spectra of 4-Cl-3-CF₃-chalcone-N₃ (K1)

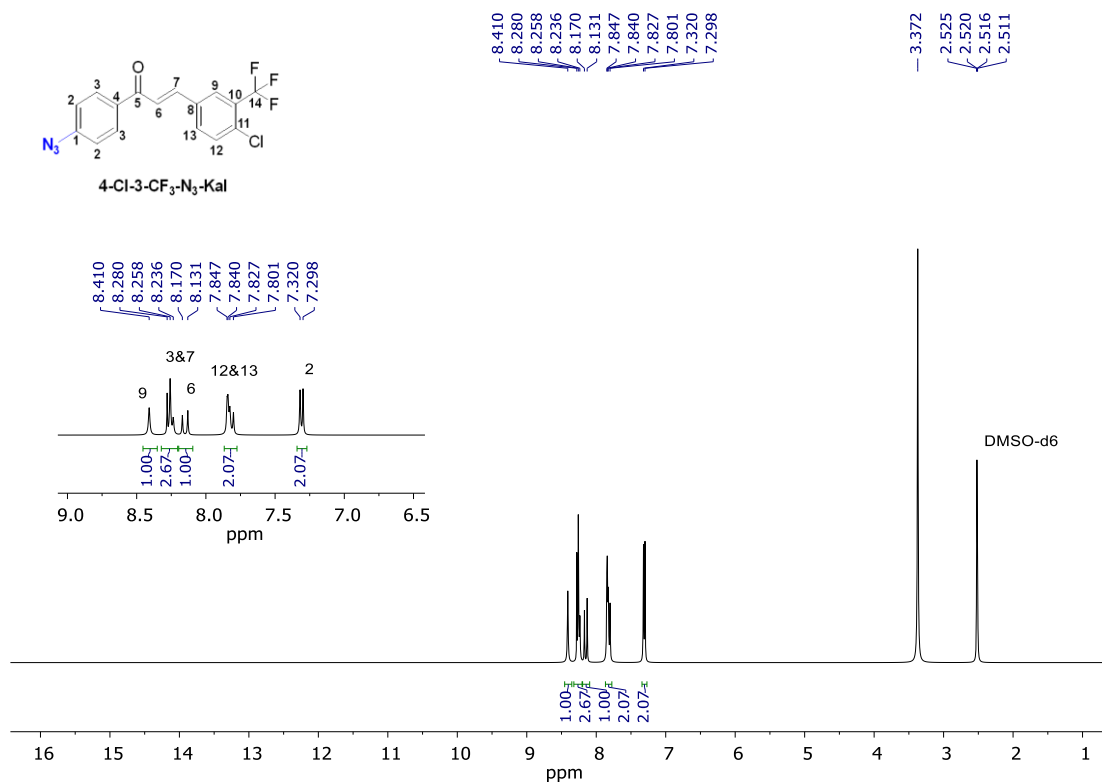


Figure S5. ¹H-NMR spectra of 4-Cl-3-CF₃-chalcone-N₃ (DMSO-d₆) (K1)

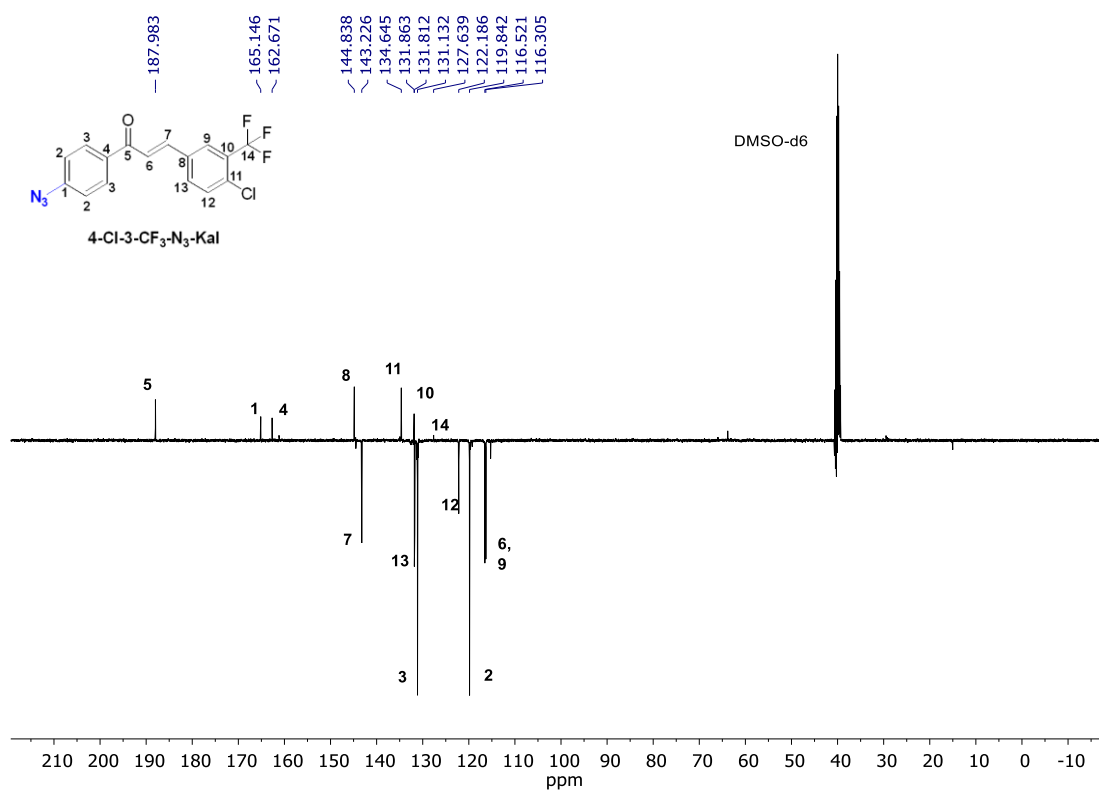


Figure S5. ¹³C-APT NMR spectra of 4-Cl-3-CF₃-chalcone-N₃ (DMSO-d₆) (K1)

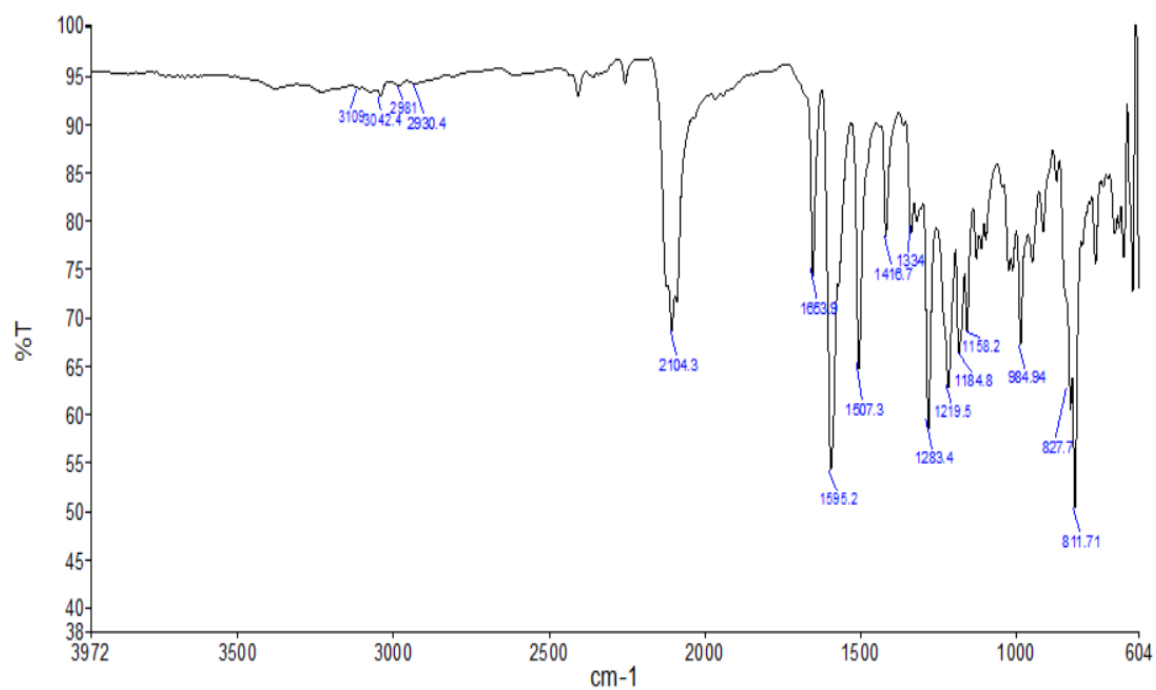


Figure S6. FT-IR (ATR) spectra of 4-F-chalcone-N₃-Kal (K2)

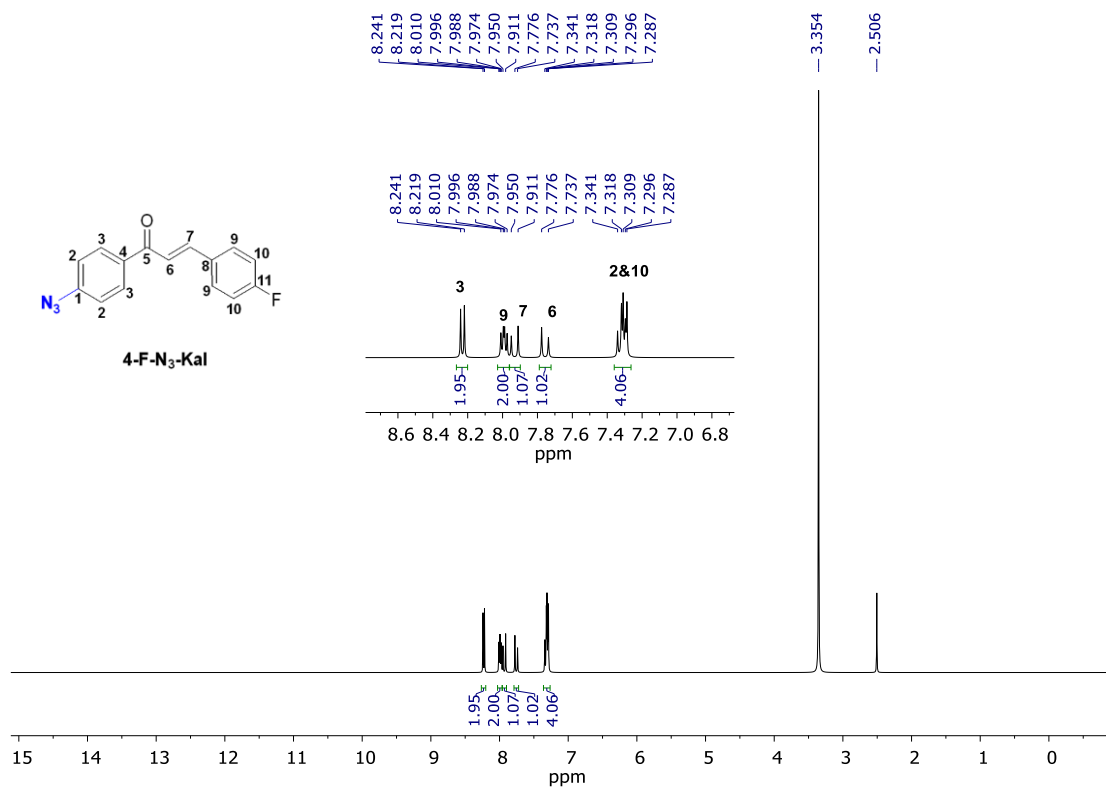


Figure S7. ¹H-NMR spectra of 4-F-chalcone-N₃ (K2) (DMSO-d₆)

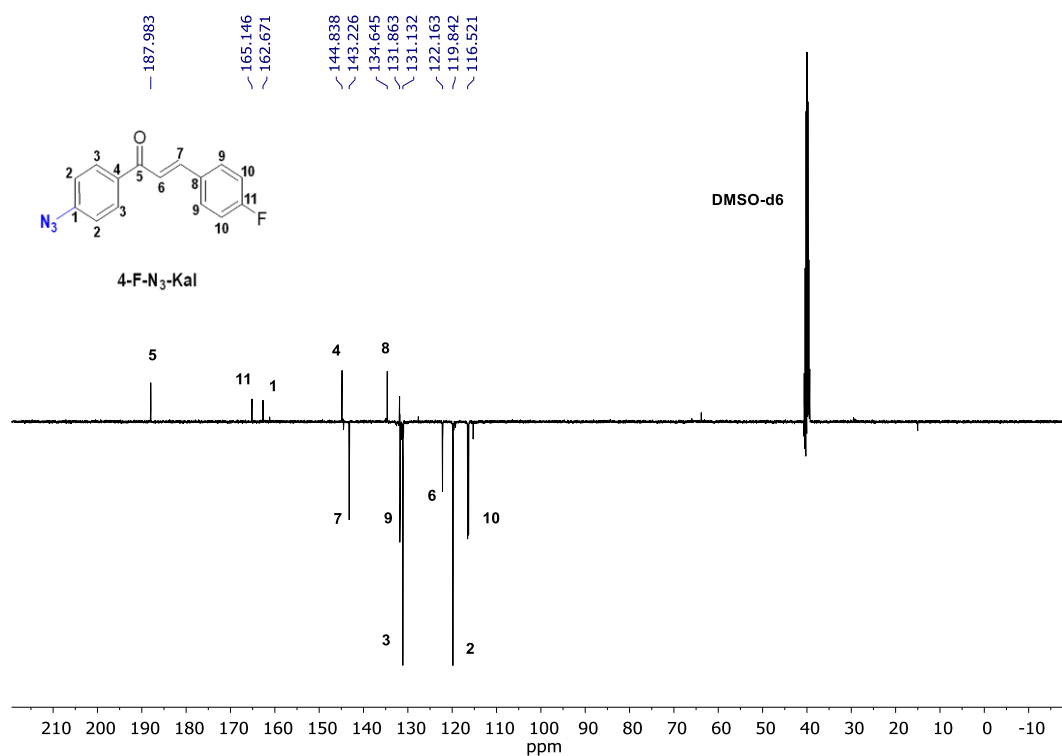


Figure S8. ¹³C-APT NMR spectra of 4-F-N₃-Kal (DMSO-d₆) (K2)

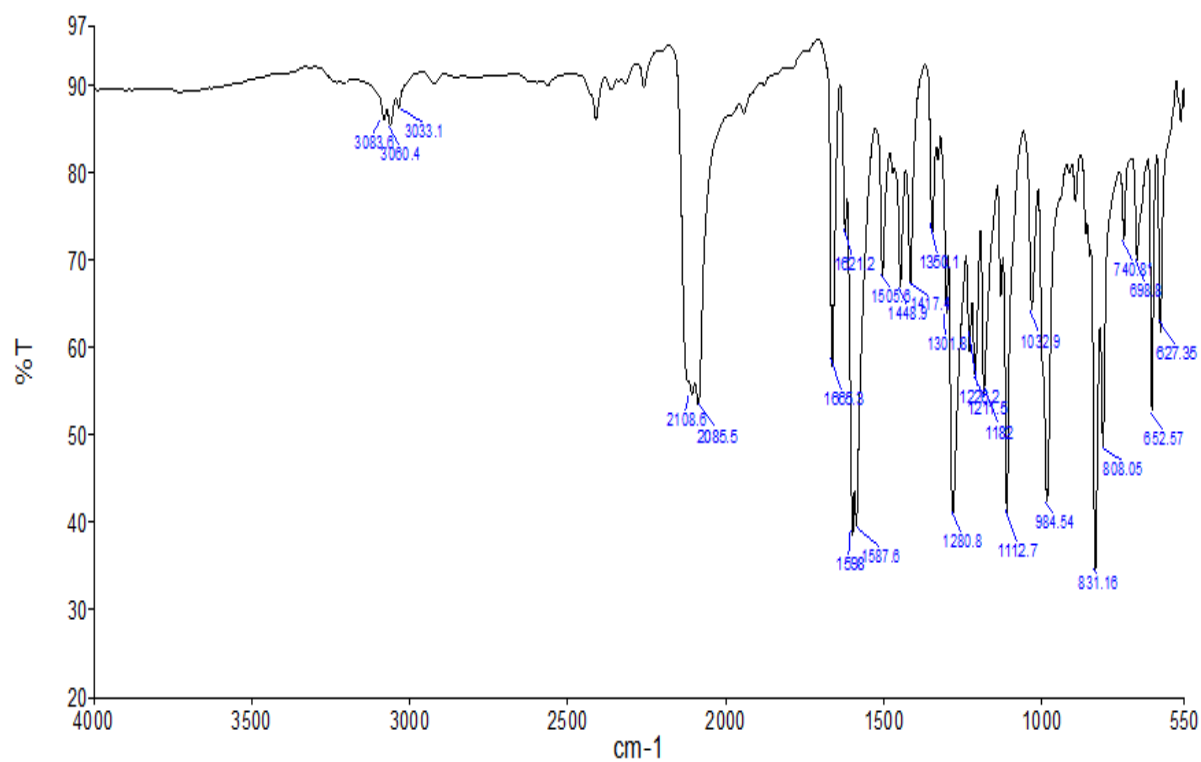


Figure S9. FT-IR (ATR) spectra of 3,5-DiF-chalcone-N₃ (K3)

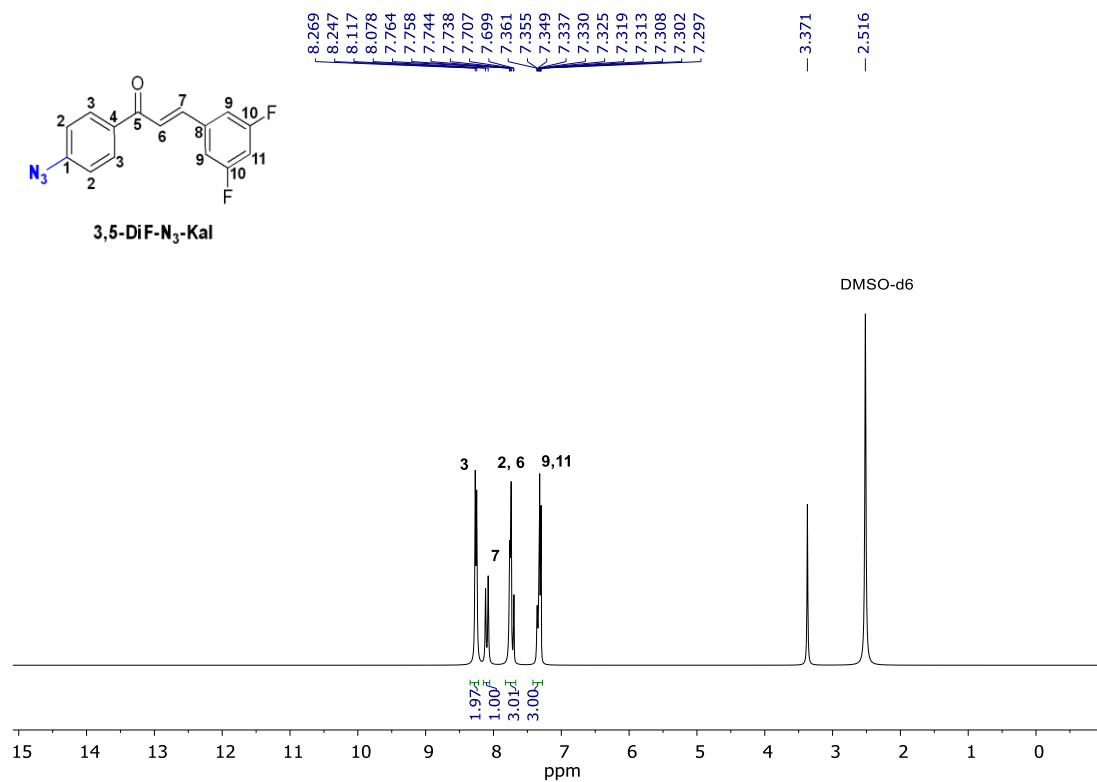


Figure S10. ¹H-NMR spectra of 3,5-DiF-chalcone-N₃ (K3) (DMSO-d₆)

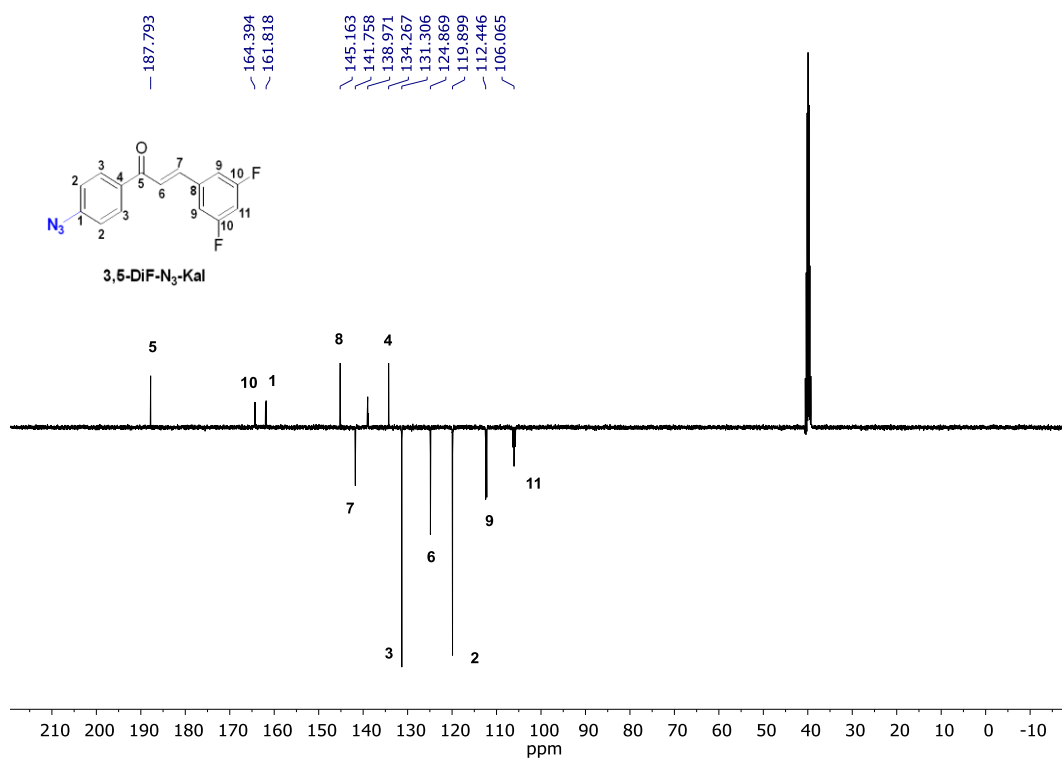


Figure S11. ¹³C-APT NMR spectra of 3,5-DiF-chalcone-N₃ (K3) (DMSO-d₆)

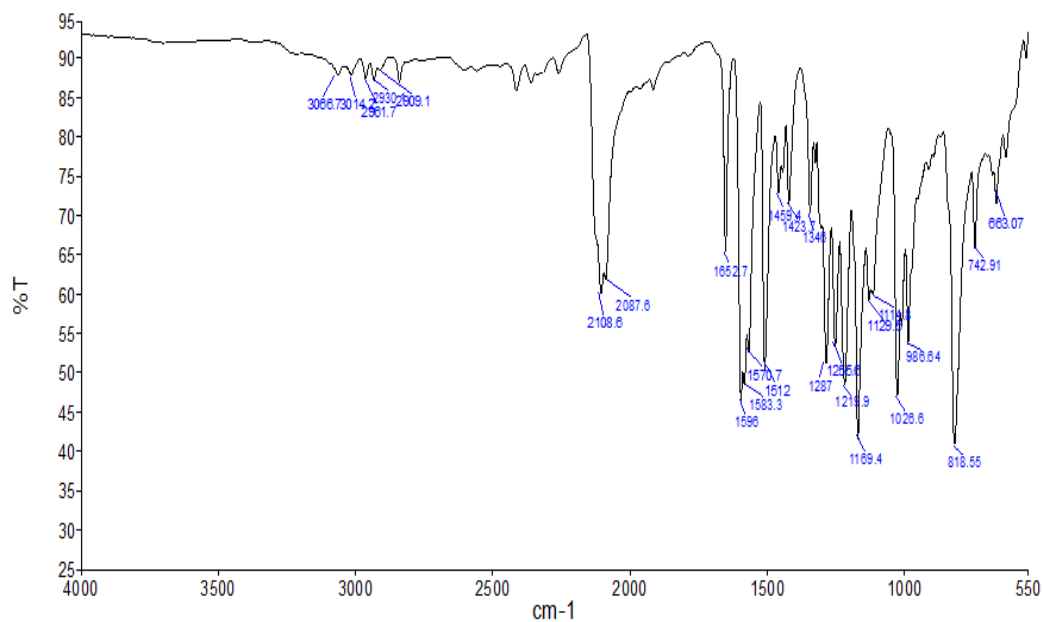


Figure S12. FT-IR (ATR) spectra of **4-OCH₃-chalcone-N₃ (K4)**

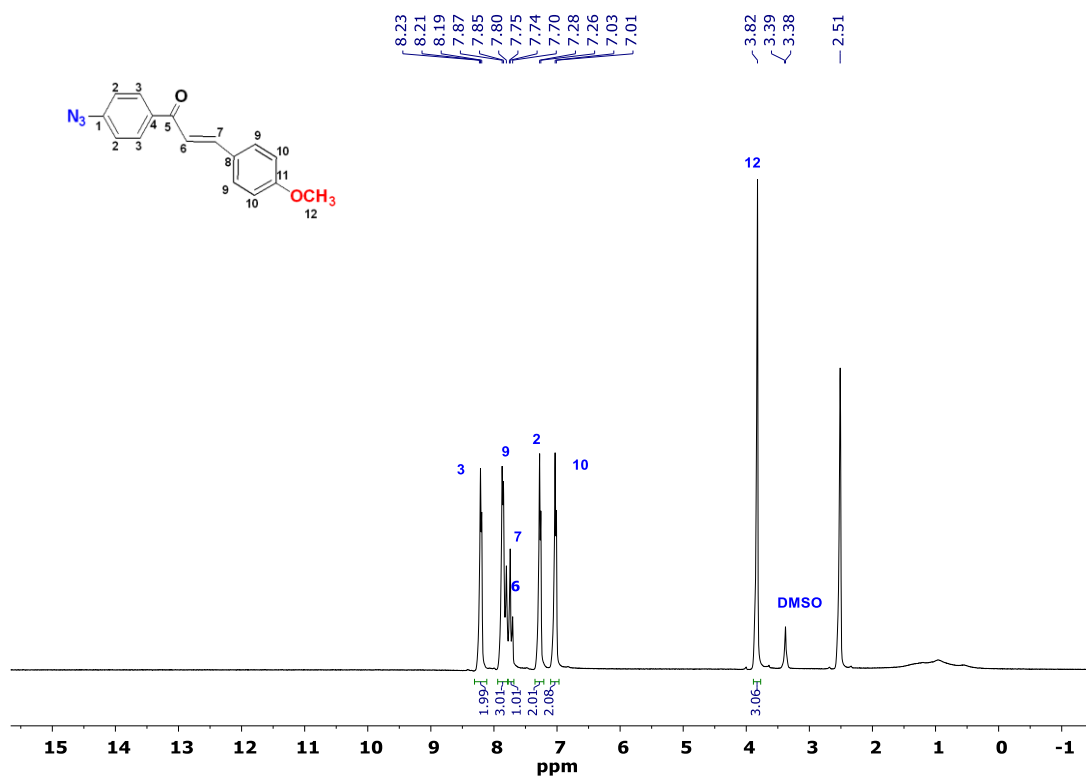


Figure S13. ¹H-NMR spectra of **4-OCH₃-chalcone-N₃ (K4)** (DMSO-d₆)

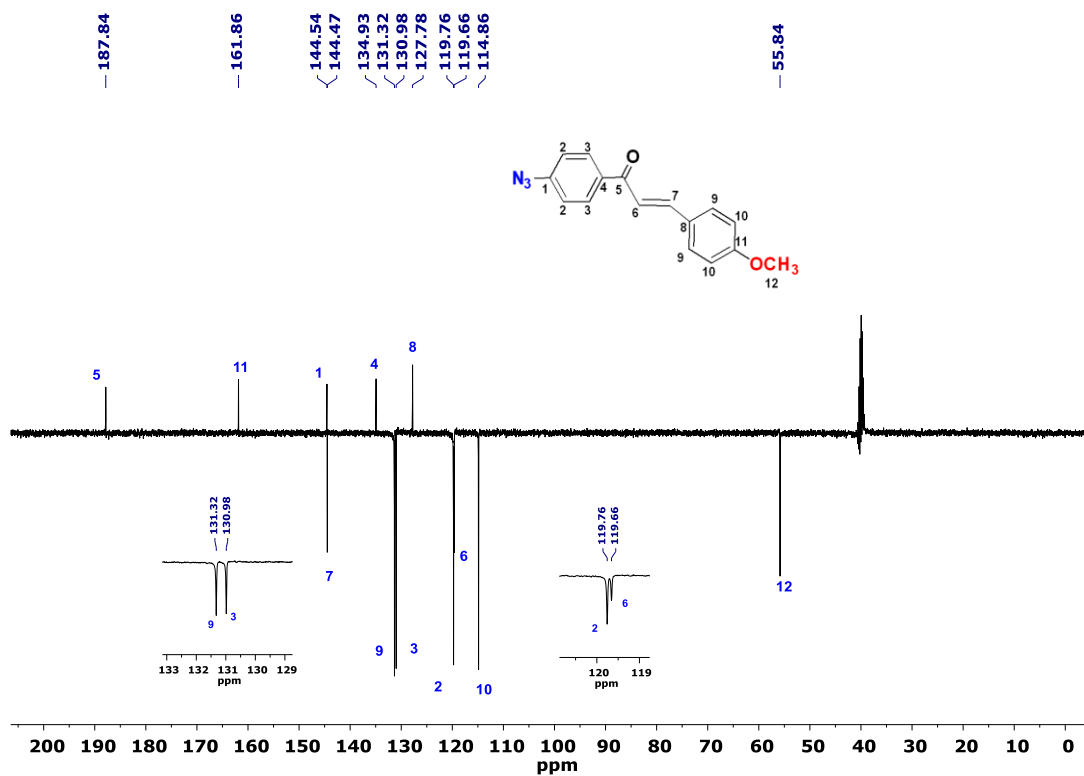


Figure S14. ¹³C-NMR spectra of *4-OCH₃-chalcone-N₃* (K4) (DMSO-d₆)

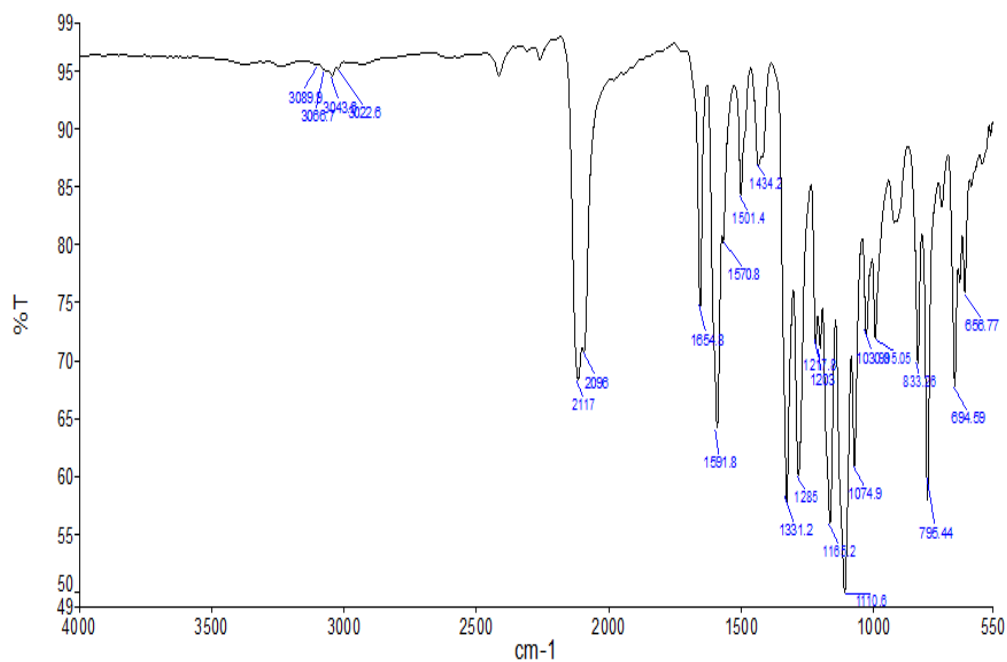


Figure S15. FT-IR (ATR) spectra of *3-CF₃-chalcone-N₃* (K5)

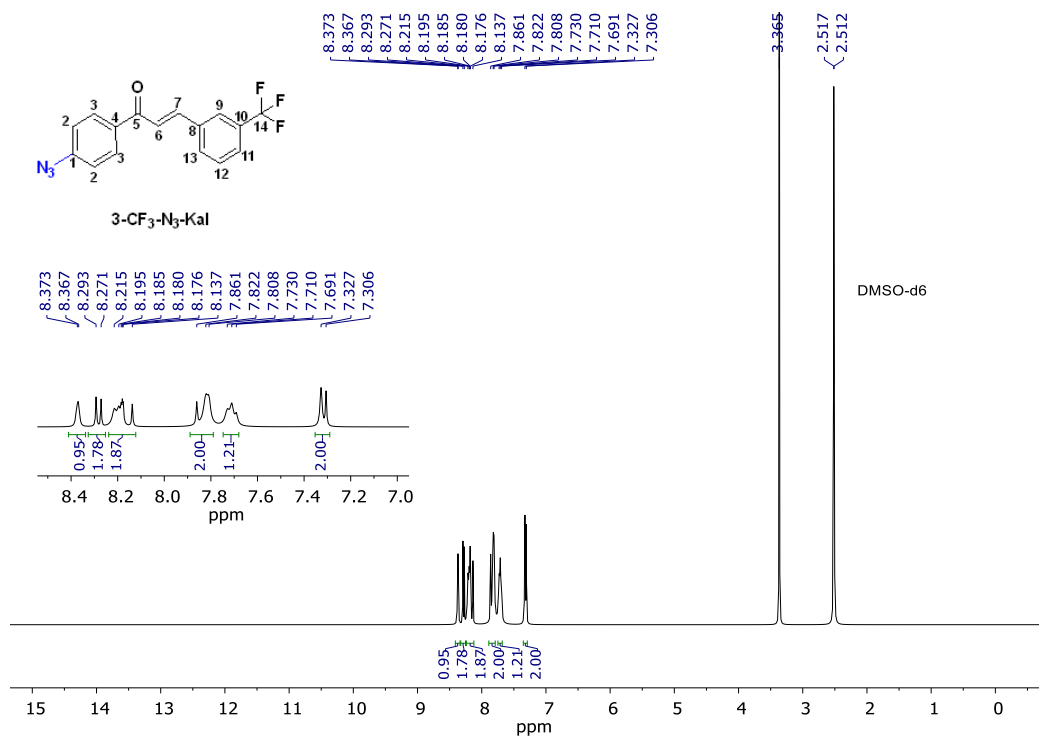


Figure S16. ¹H-NMR spectra of 3-CF₃-chalcone-N₃ (K5) (DMSO-d₆)

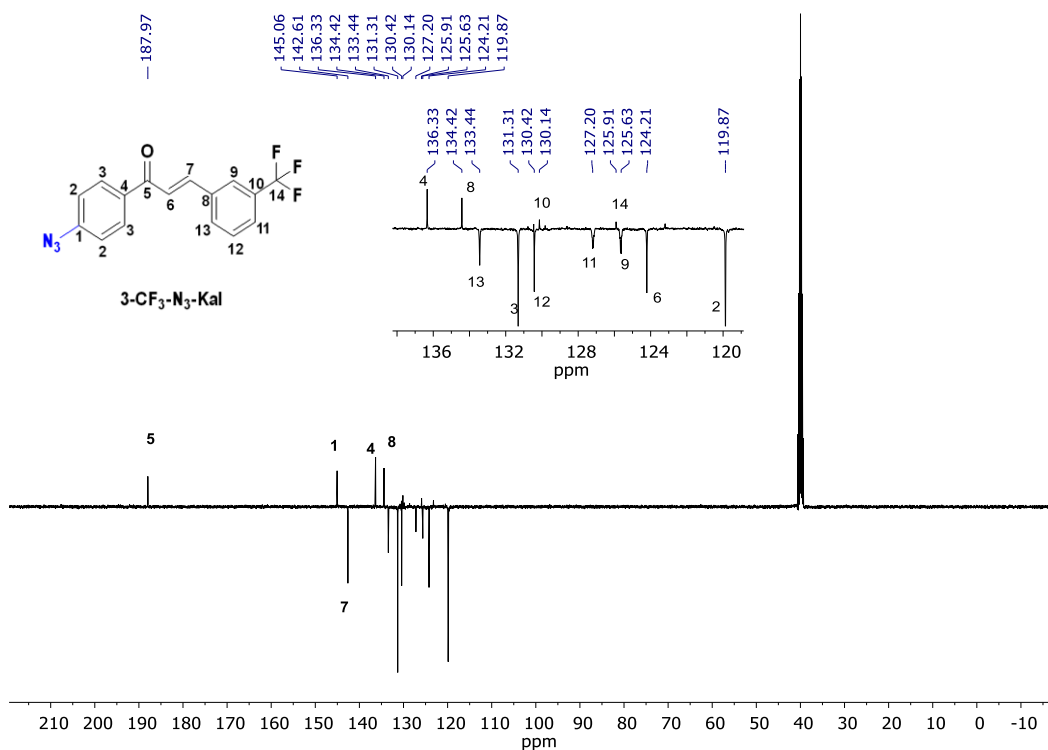


Figure S17. ¹³C-NMR spectra of 3-CF₃-chalcone-N₃ (K5) (DMSO-d₆)

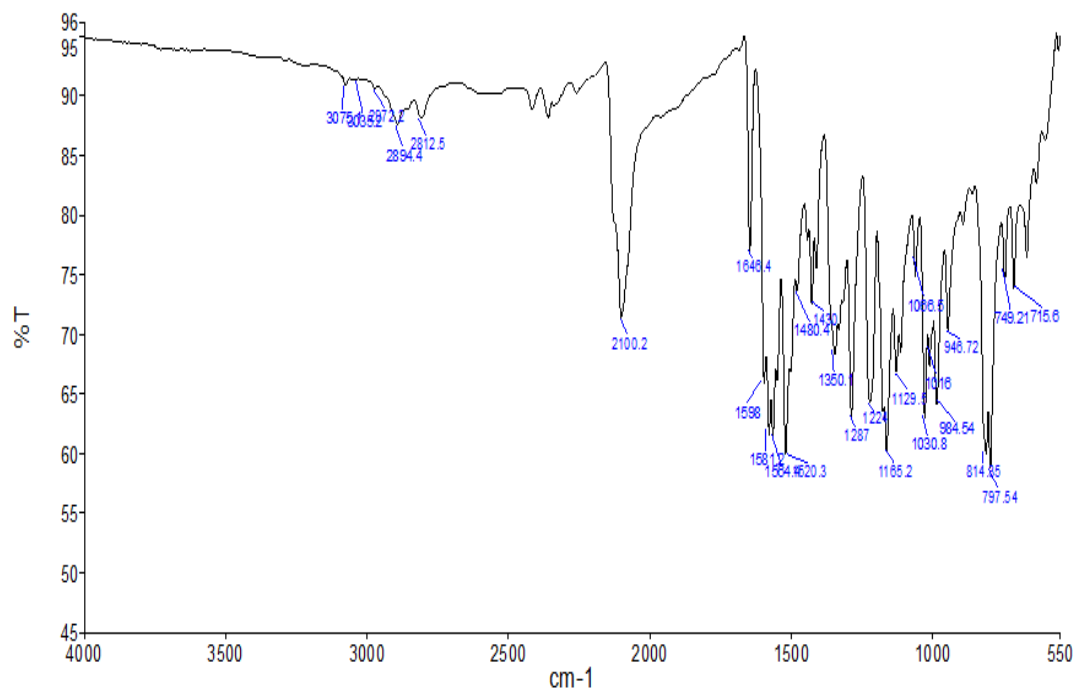


Figure S18. FT-IR (ATR) spectra of *4-N(CH₃)₂-chalcone-N₃ (K6)*

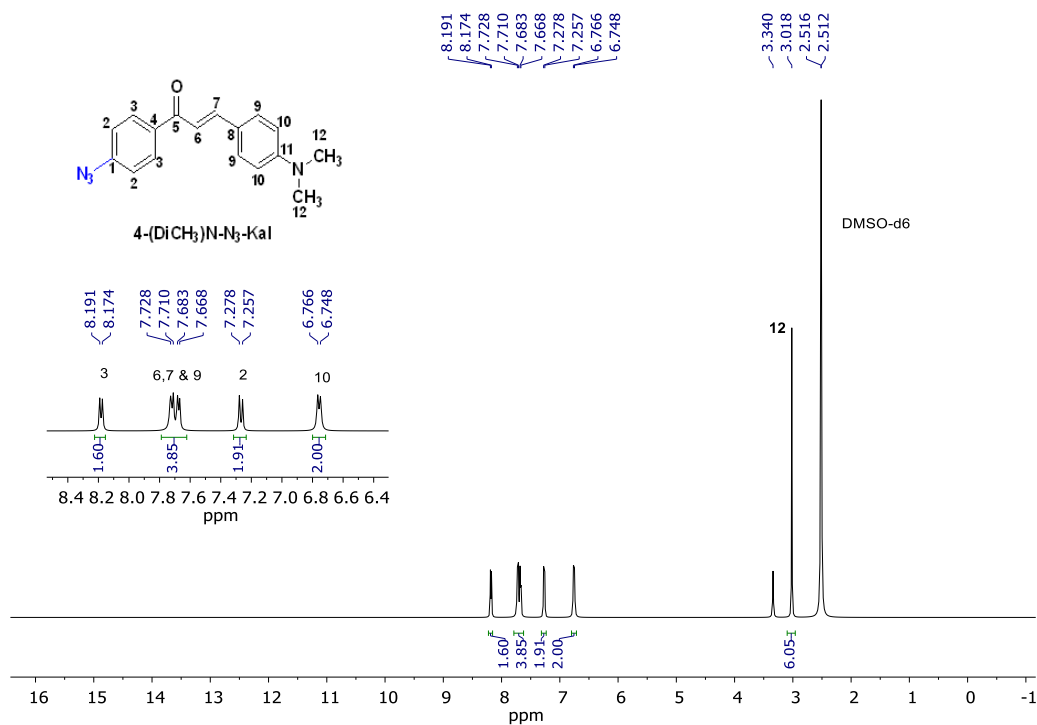


Figure S19. ¹H-NMR spectra of *4-N(CH₃)₂-chalcone-N₃ (K6)* (DMSO-d₆)

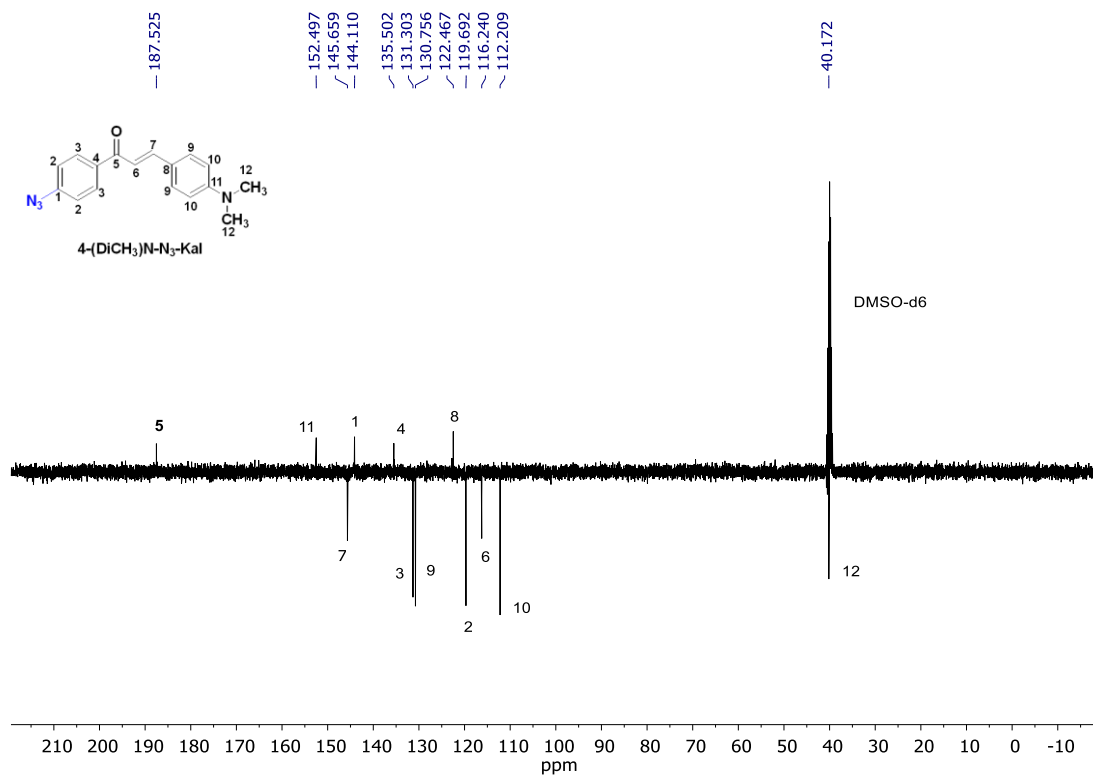


Figure S20. ¹³C-NMR spectra of 4-*N*(CH₃)₂-chalcone-*N*₃ (K6) (DMSO-d₆)

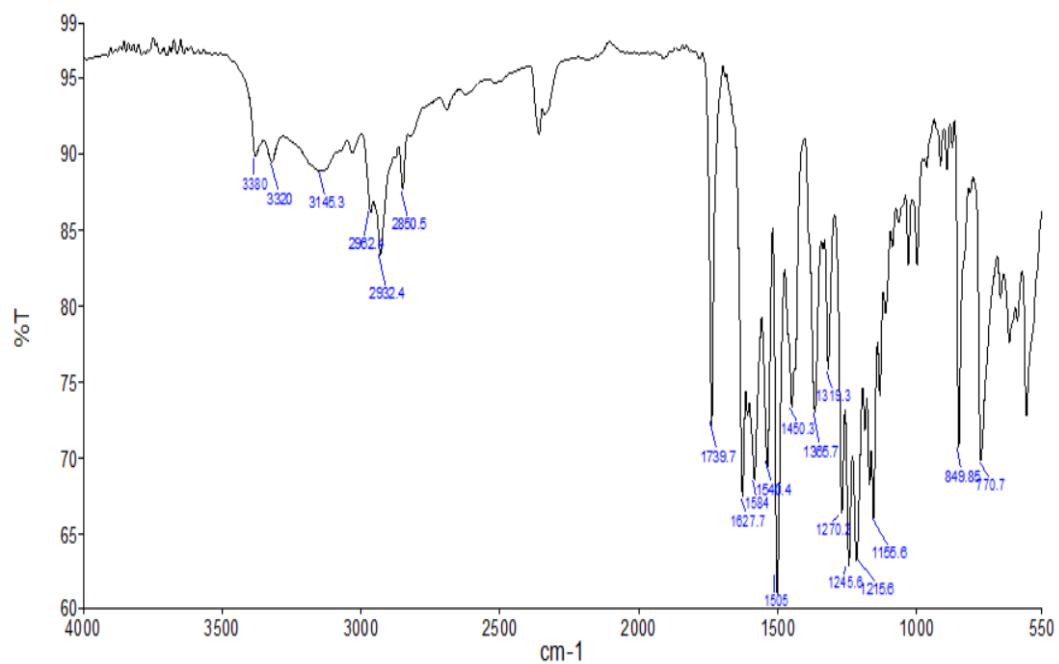


Figure S21. FT-IR (ATR) spectra of OH-Bnz-Val-OCH₃

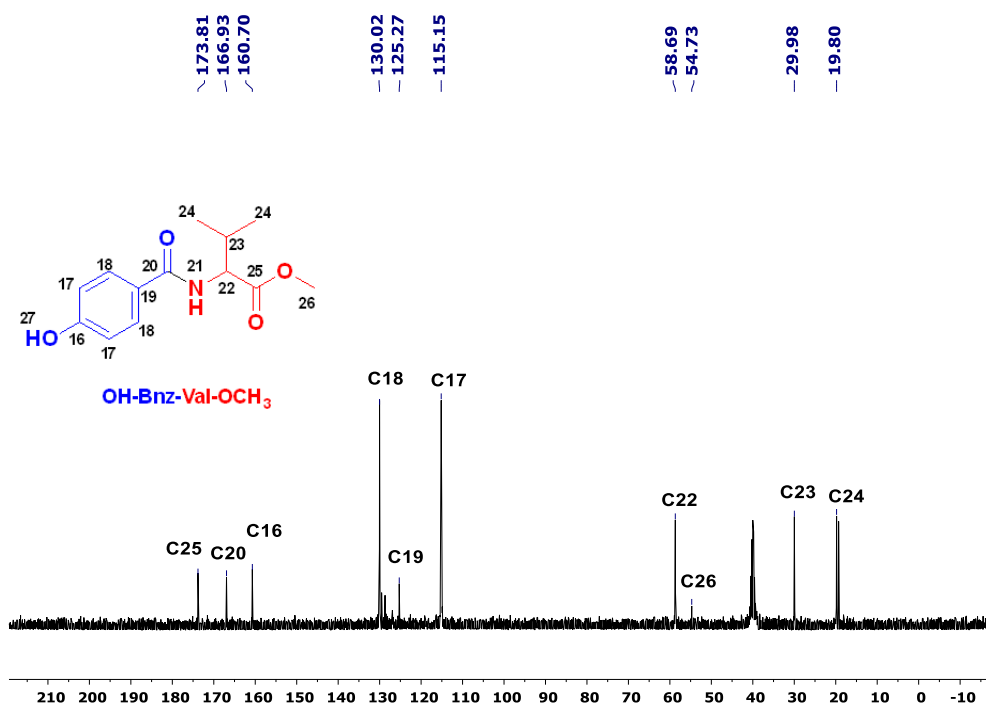
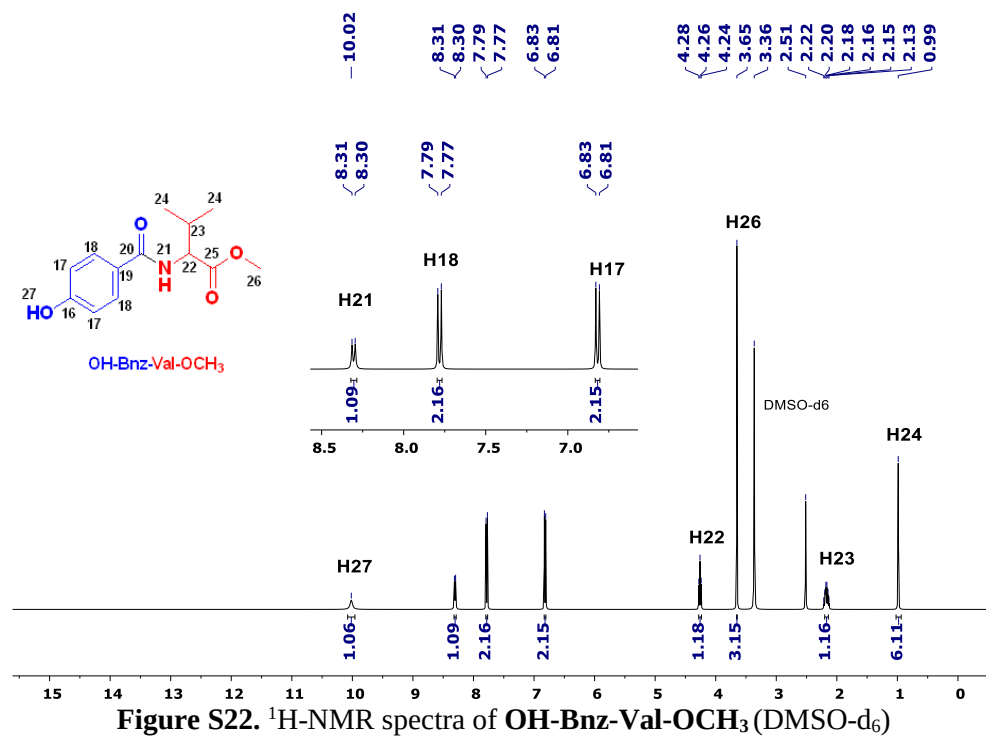


Figure S23. ¹³C-NMR spectra of OH-Bnz-Val-OCH₃ (DMSO-d₆)

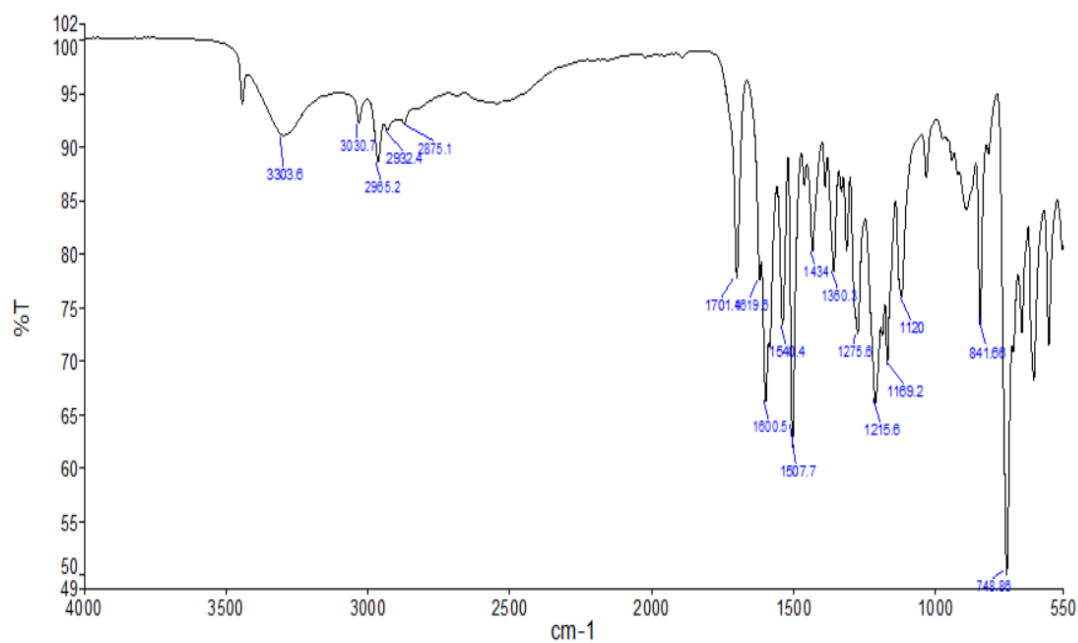


Figure S4. FT-IR (ATR) spectra of OH-Bnz-Val-OH

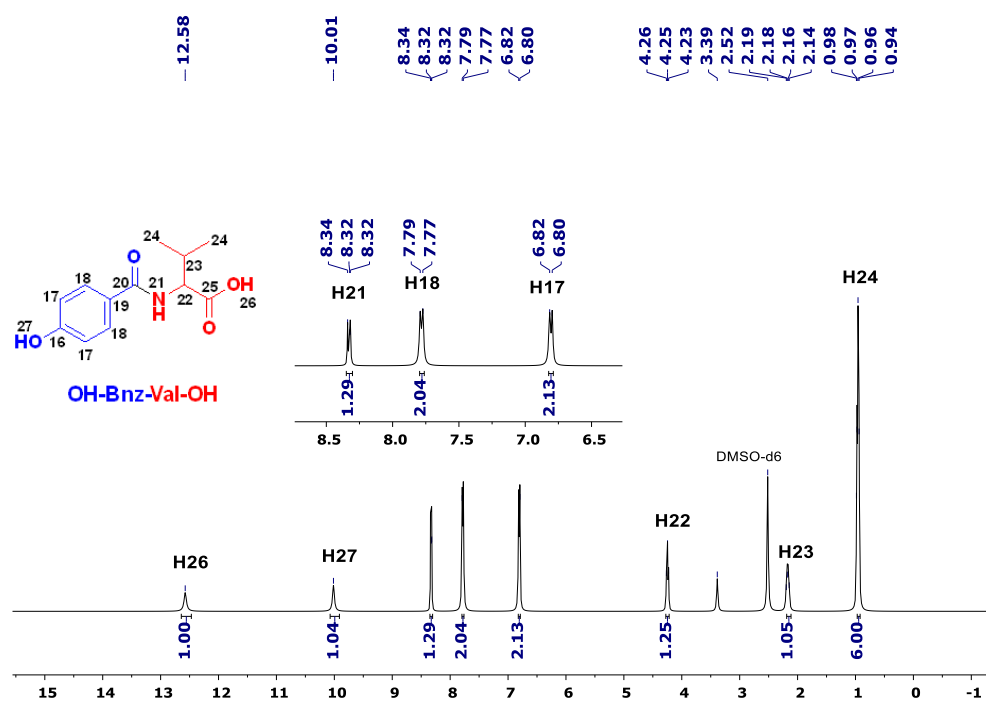


Figure S25. ¹H-NMR spectra of OH-Bnz-Val-OH (DMSO-d₆)

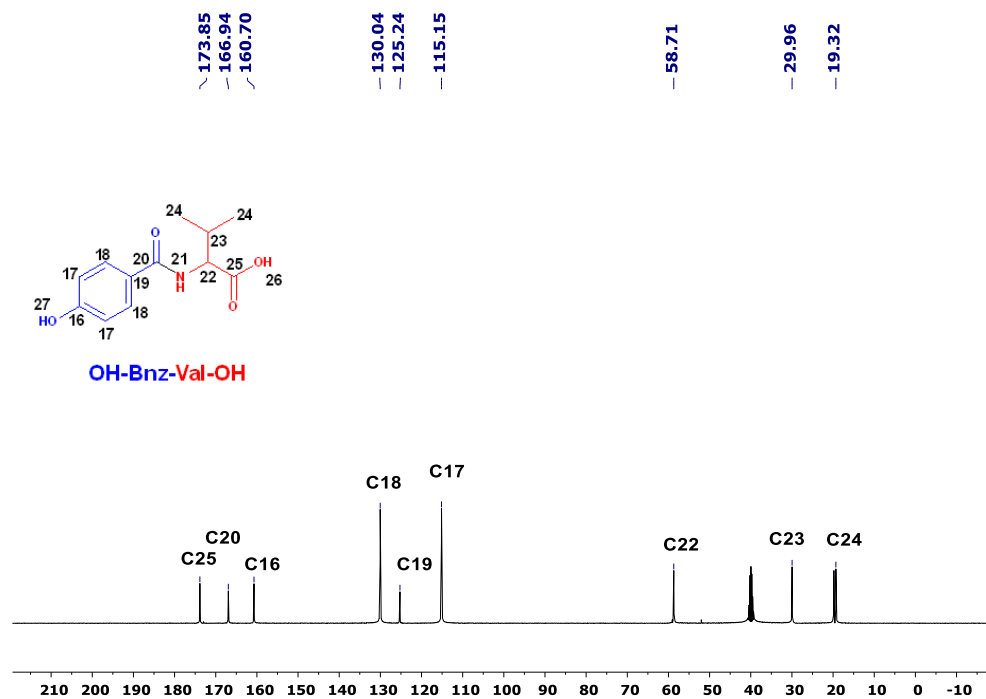


Figure S26. ¹³C-NMR spectra of OH-Bnz-Val-OH (DMSO-d₆)

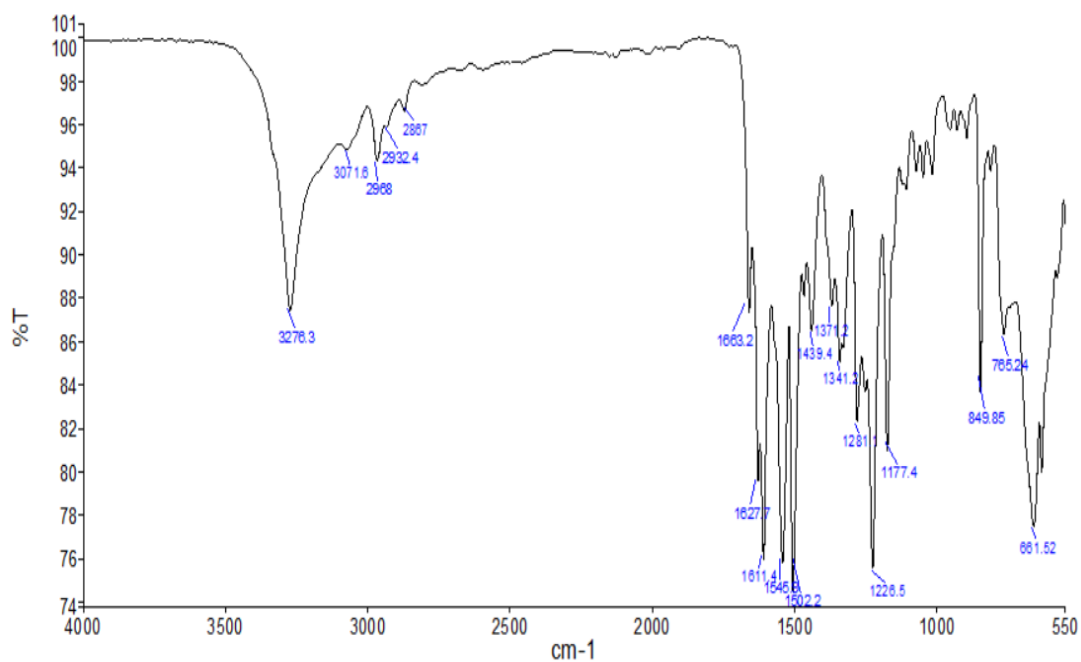
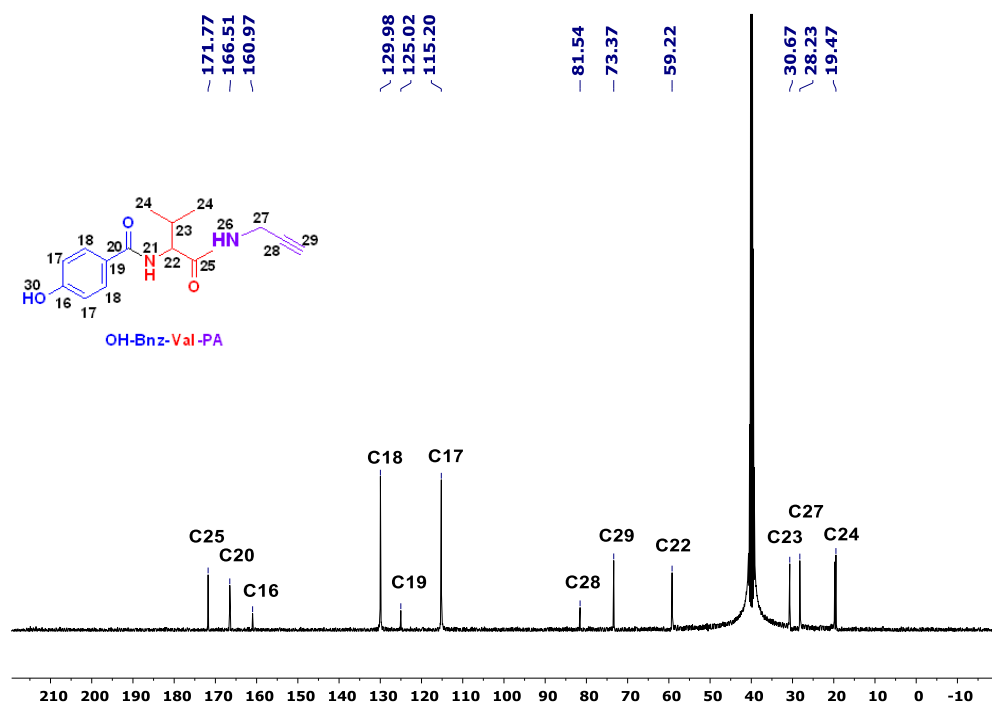
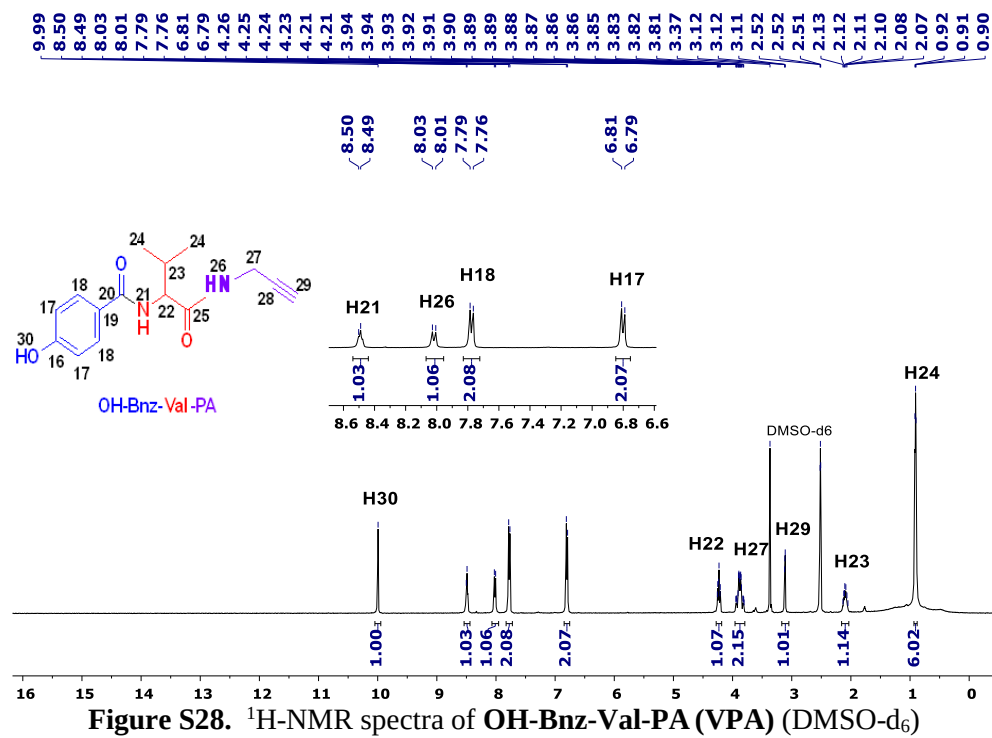


Figure S27. FT-IR (ATR) spectra of OH-Bnz-Val-PA (VPA)



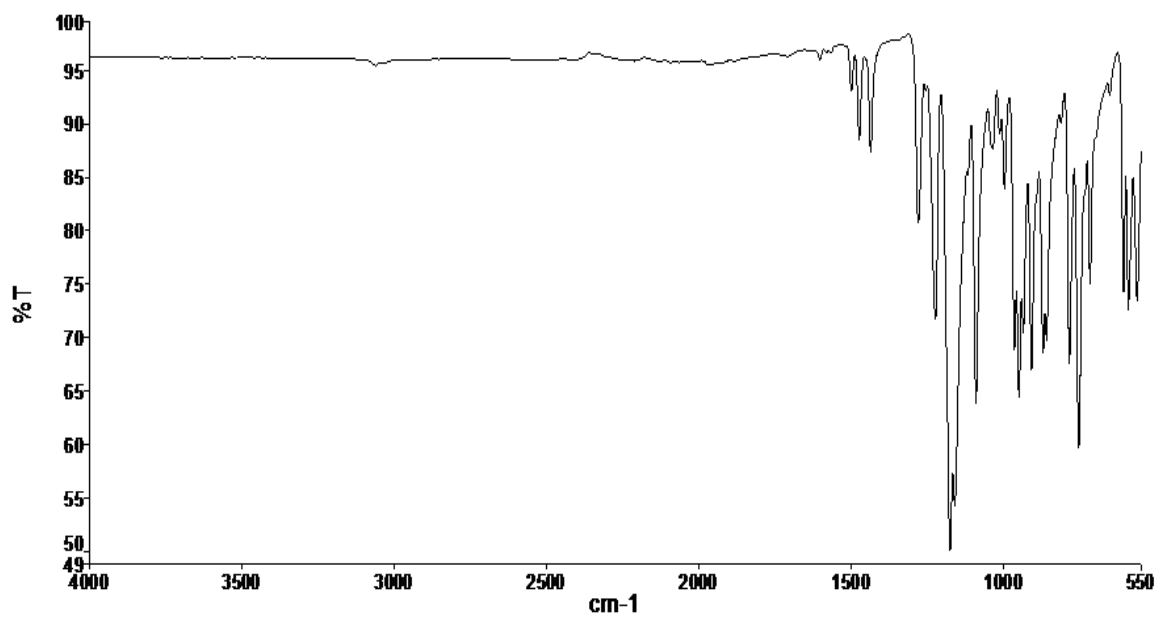


Figure S30. FT-IR (ATR) spectra of **DPP**

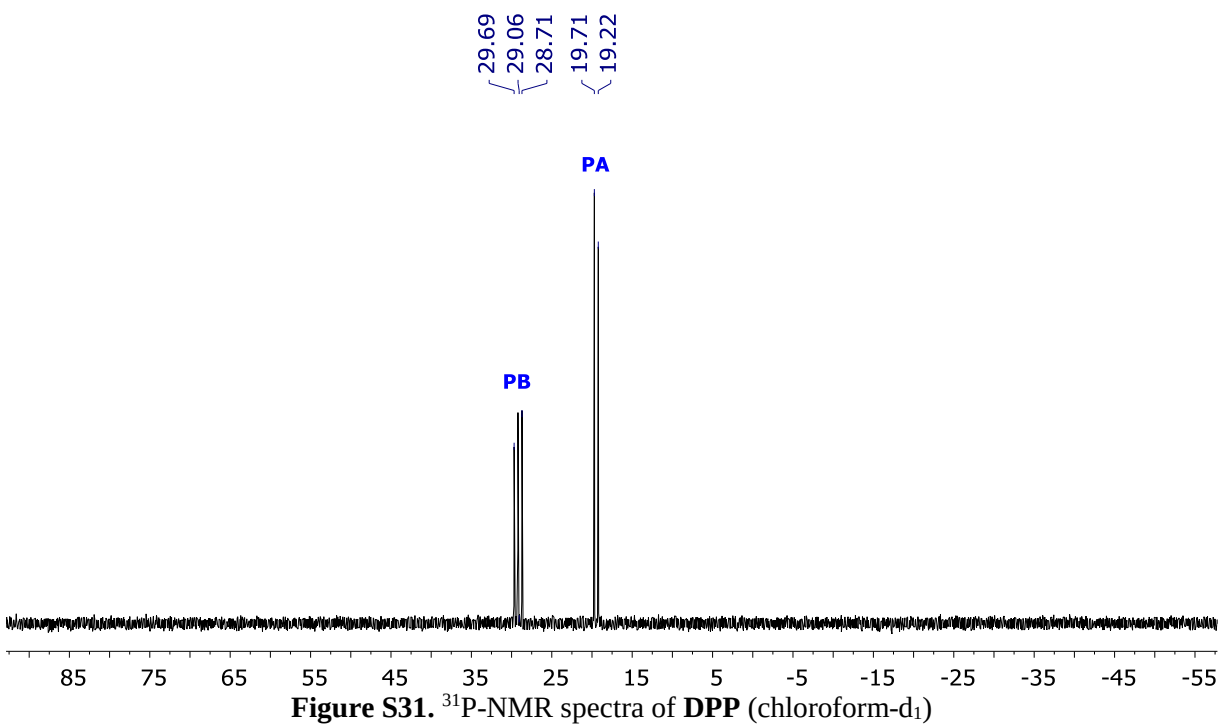


Figure S31. ^{31}P -NMR spectra of **DPP** (chloroform- d_1)

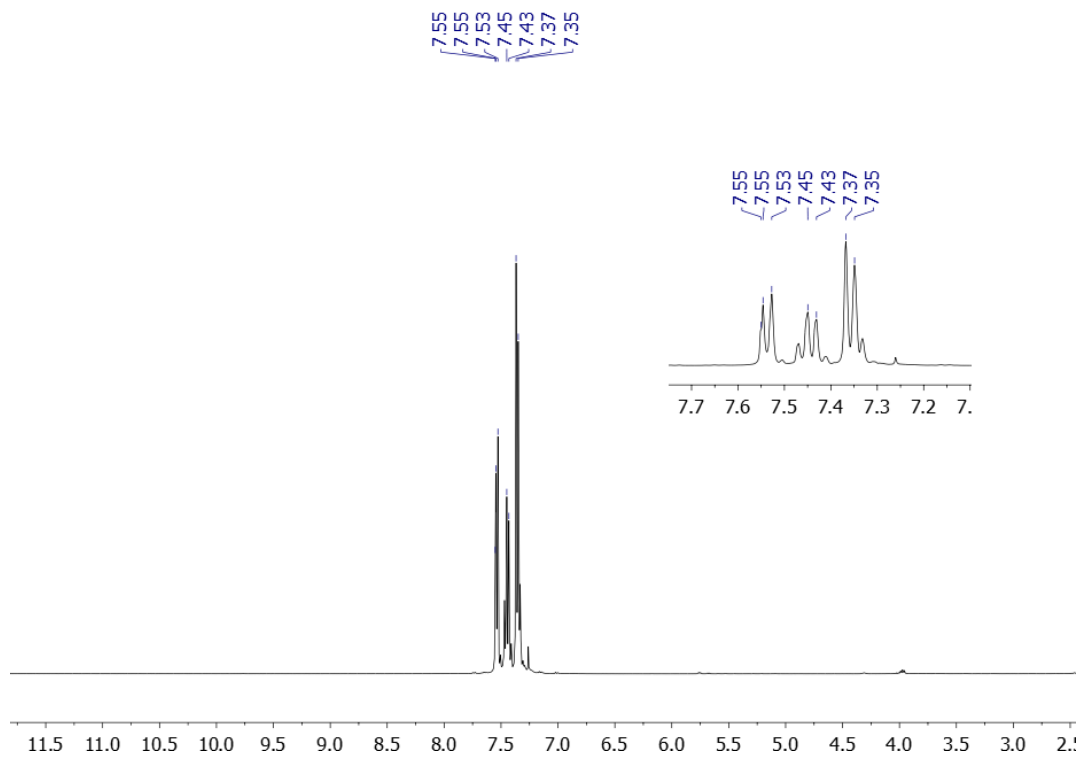


Figure S32. ^1H -NMR spectra of **DPP** (chloroform- d_1)

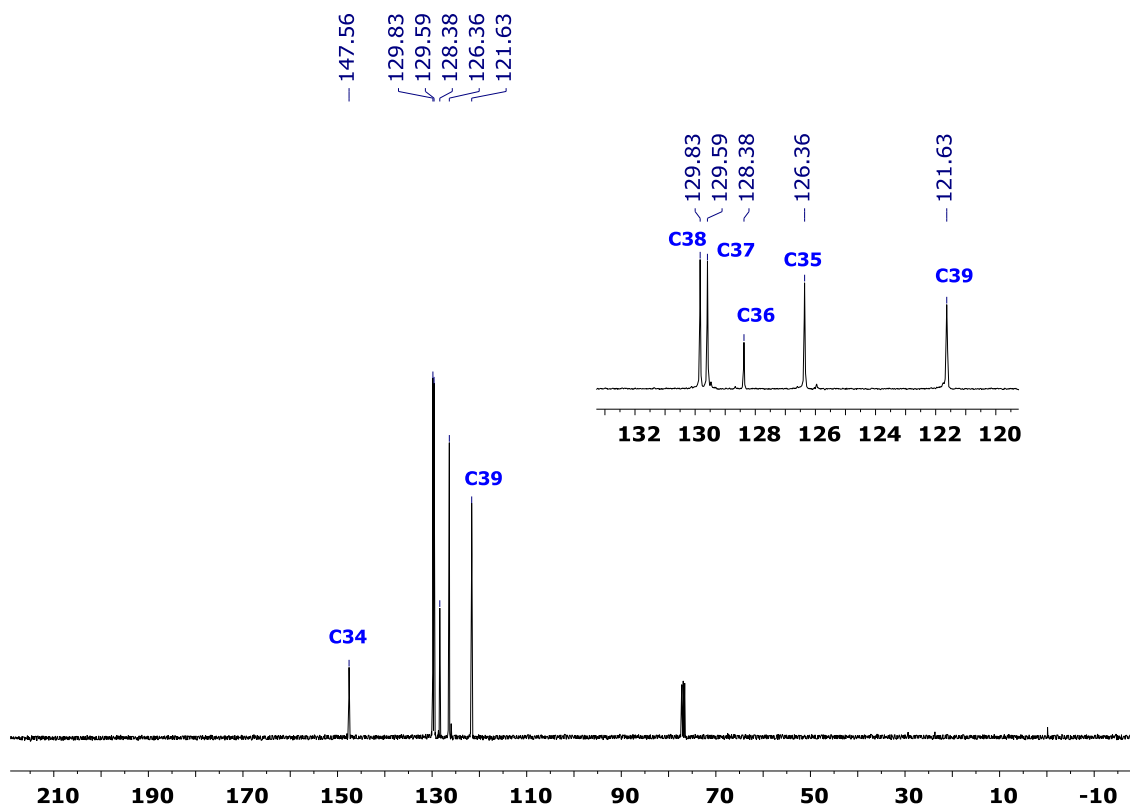


Figure S33. ^{13}C -NMR spectra of **DPP** (chloroform- d_1)

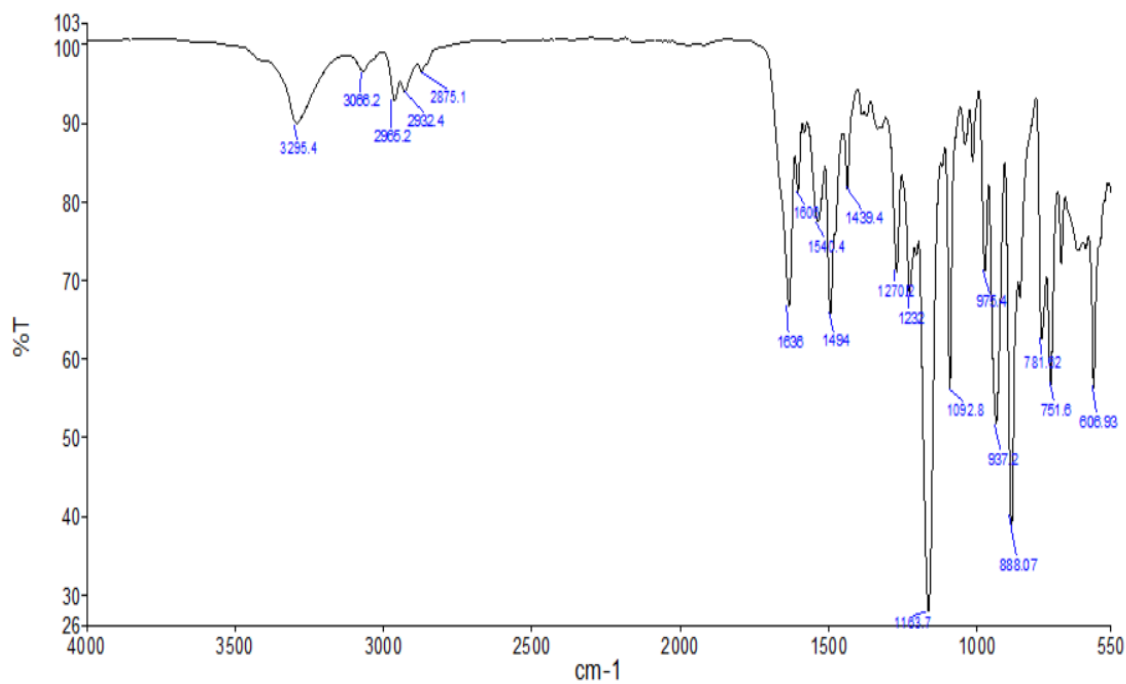


Figure S34. FT-IR (ATR) spectra of DPP-Bnz-Val-PA (BV)

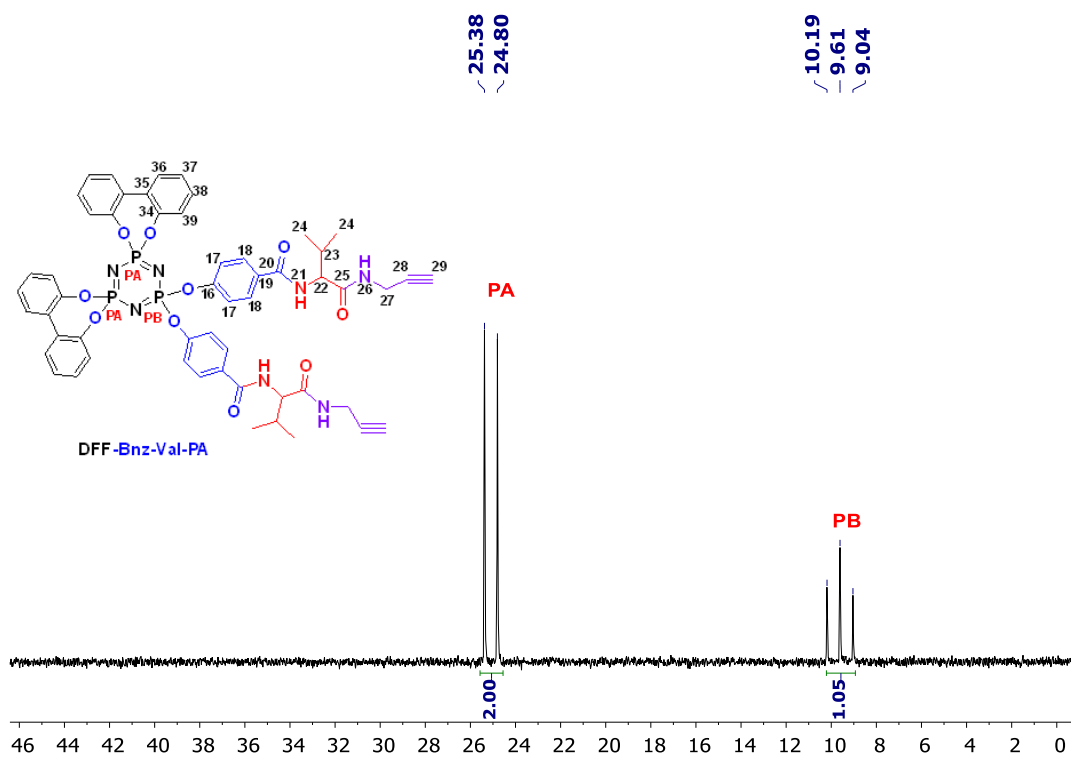


Figure S35. ³¹P-NMR spectra of DPP-Bnz-Val-PA (BV) (DMSO-d₆)

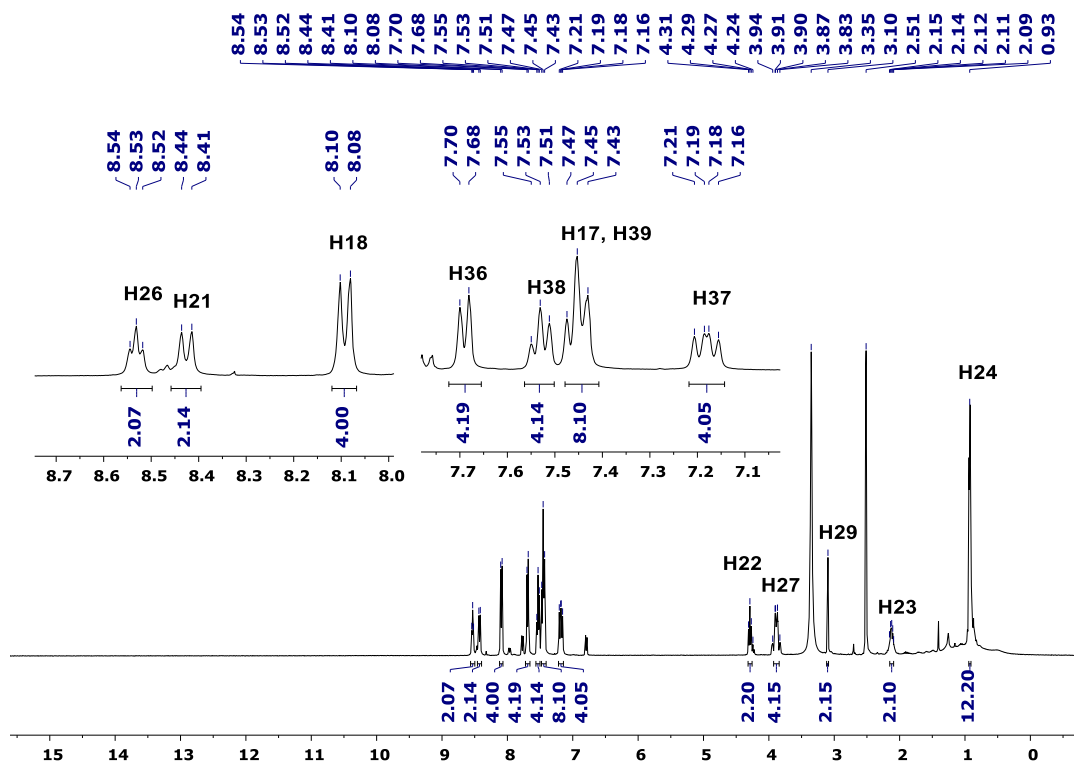


Figure S36. ^1H -NMR spectra of DPP-Bnz-Val-PA (BV) (DMSO-d_6)

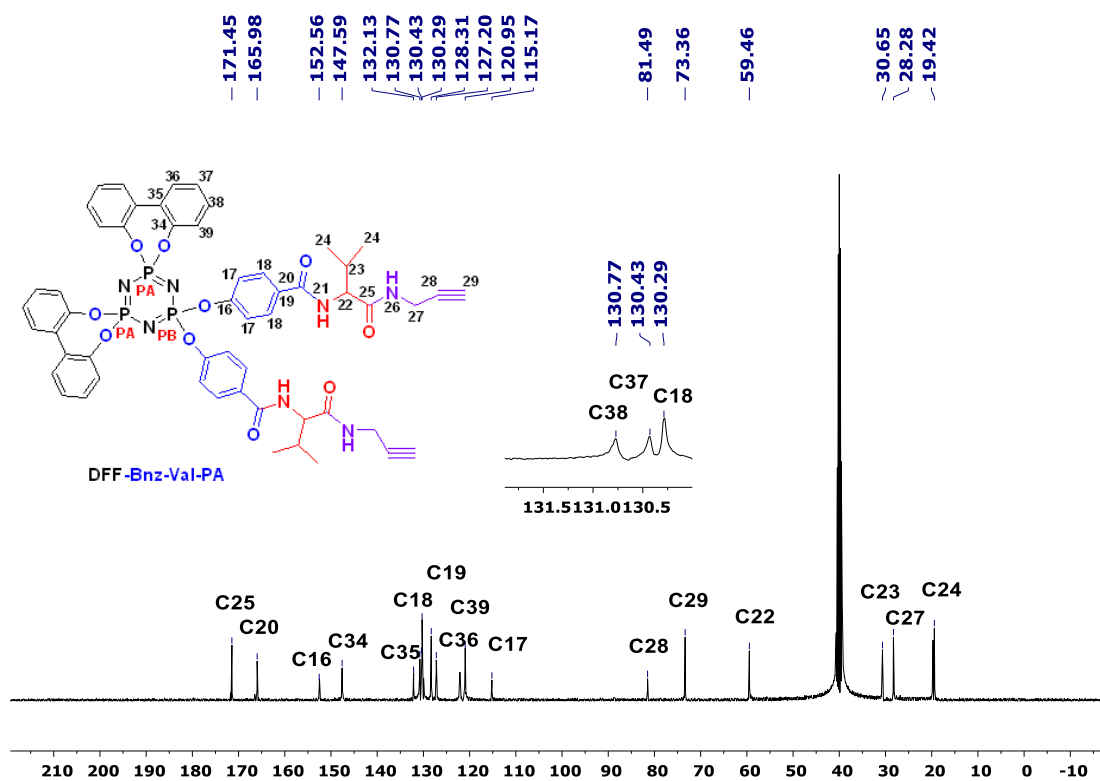


Figure S37. ^{13}C -NMR spectra of DPP-Bnz-Val-PA (BV) (DMSO-d_6)

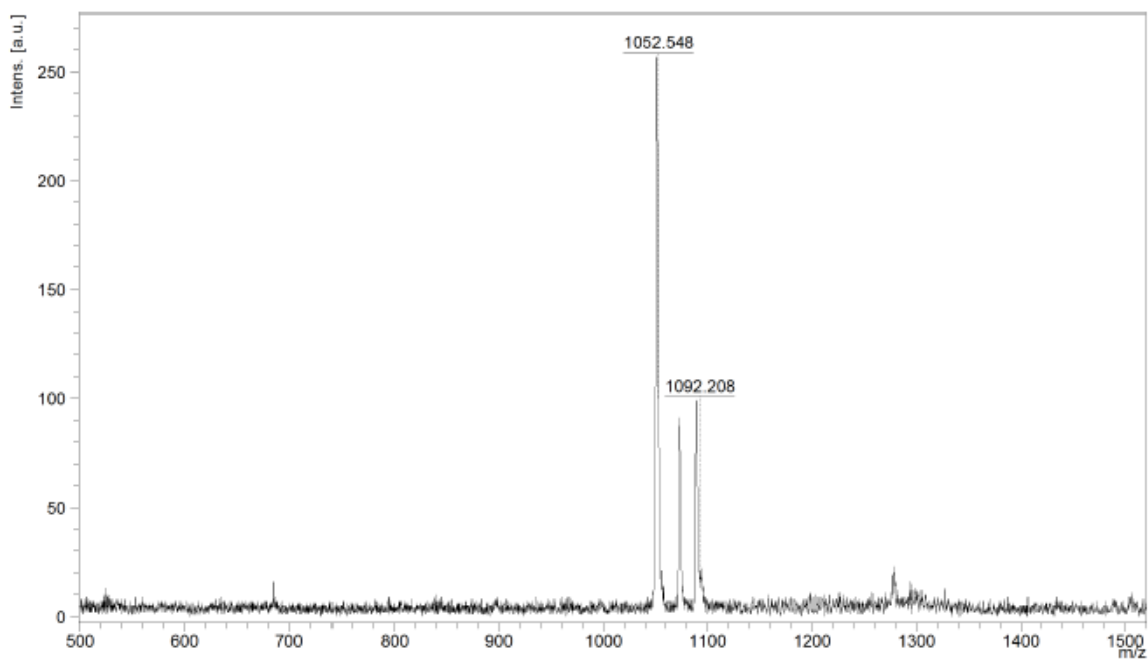


Figure S38. MALDI-TOF MS spectra of **DPP-Bnz-Val-PA (BV)**

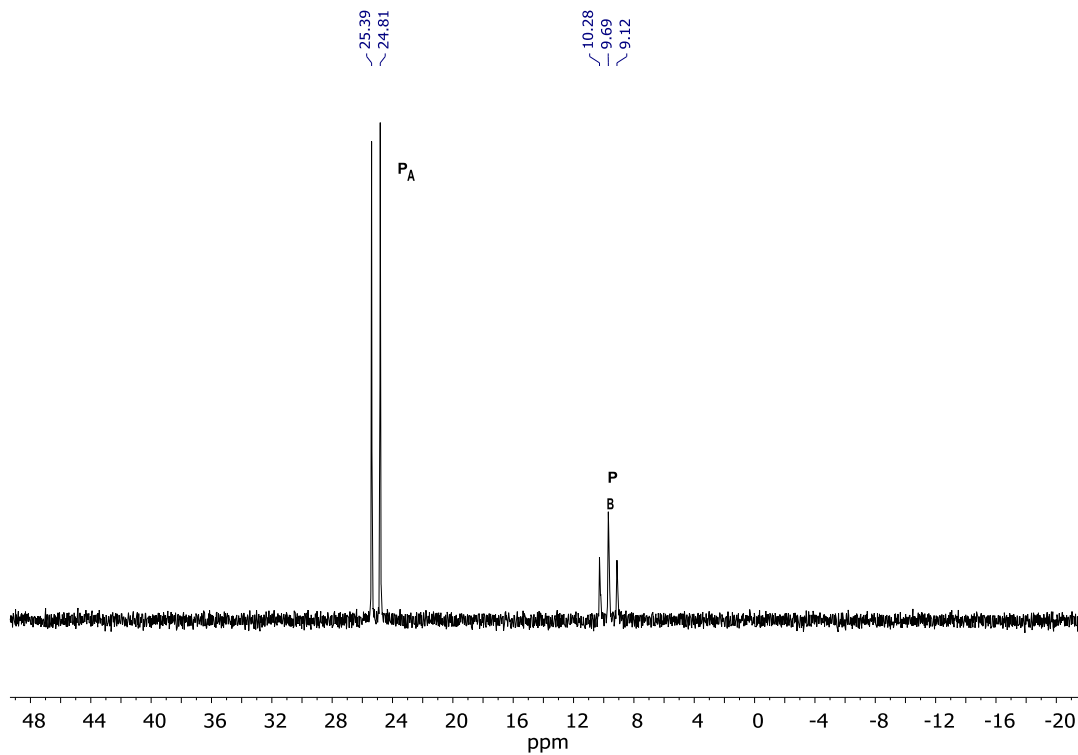


Figure S39. ³¹P-NMR spectra of **DPP-Bnz-Val-click-4-Cl-3-CF₃-chalcone (BVK1)**

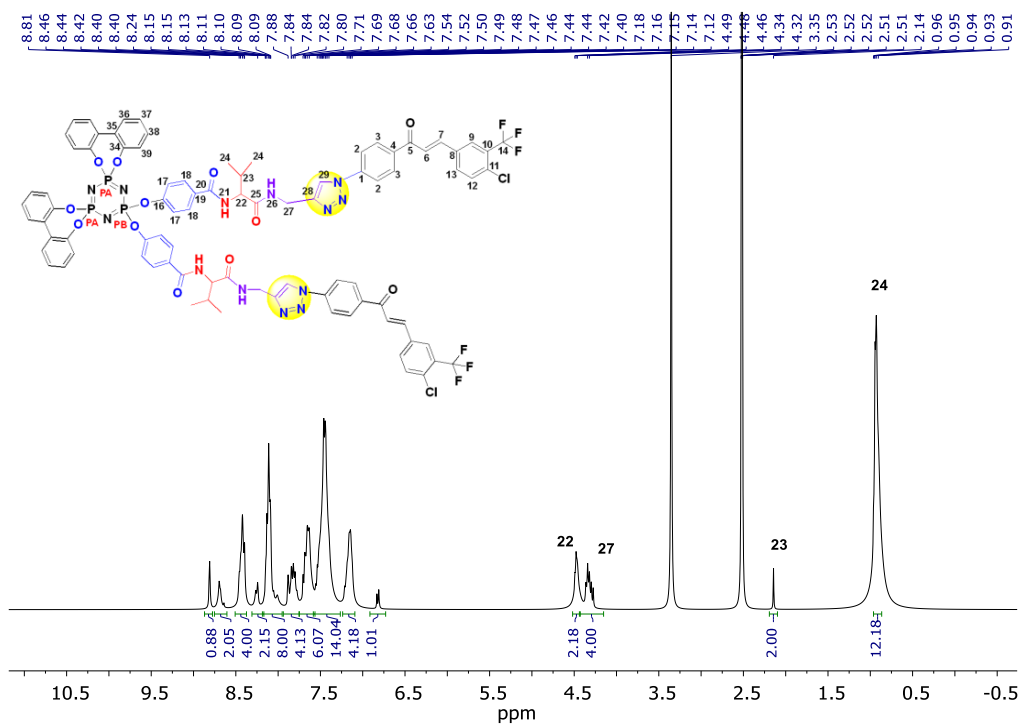


Figure S40. ¹H-NMR spectra of *DPP-Bnz-Val-click-4-Cl-3-CF₃-chalcone (BVK1)*

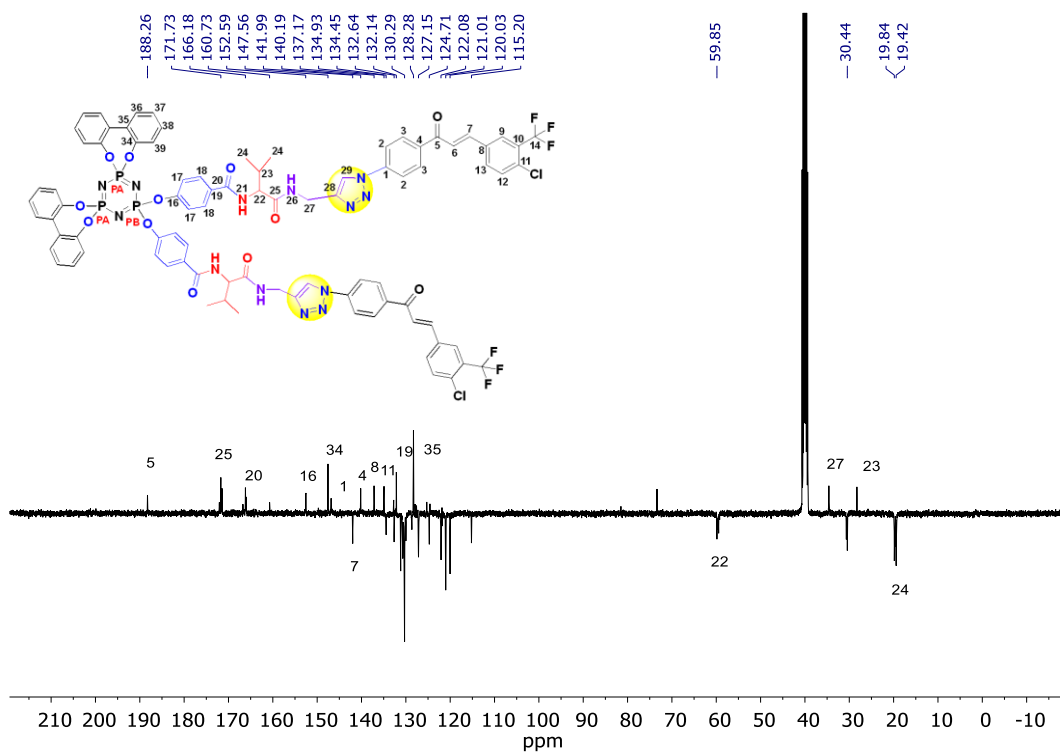


Figure S41. ¹³C-NMR spectra of *DPP-Bnz-Val-click-4-Cl-3-CF₃-chalcone (BVK1)*

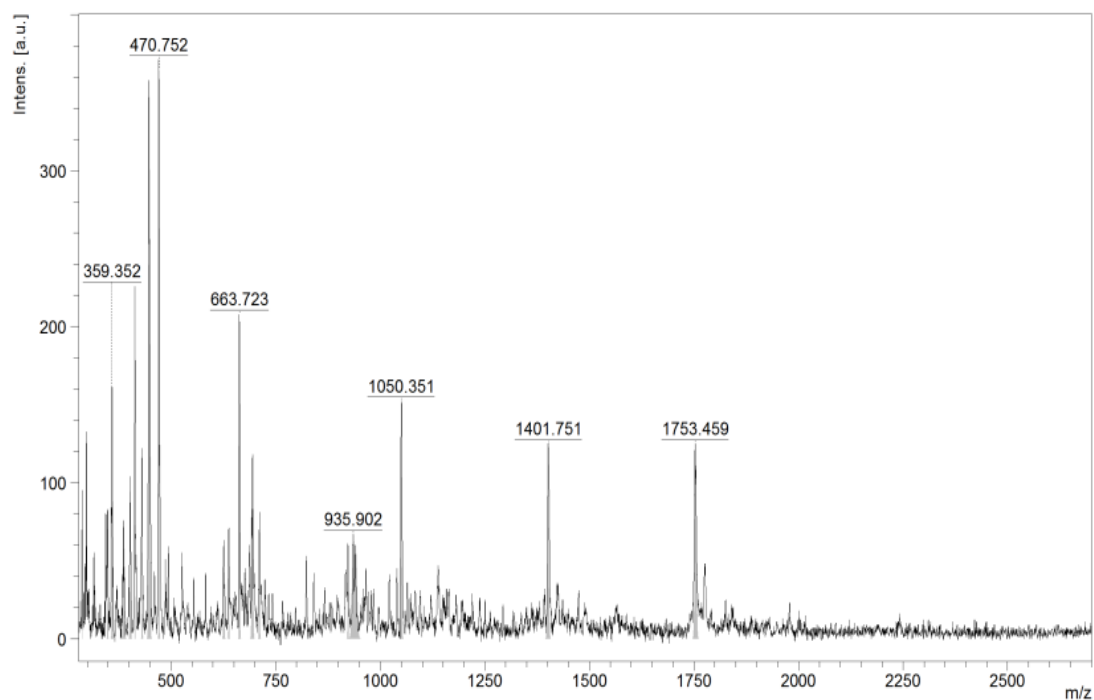


Figure S42. MALDI-TOF MS spectra of *DPP-Bnz-Val-click-4-Cl-3-CF₃-chalcone (BVK1)*

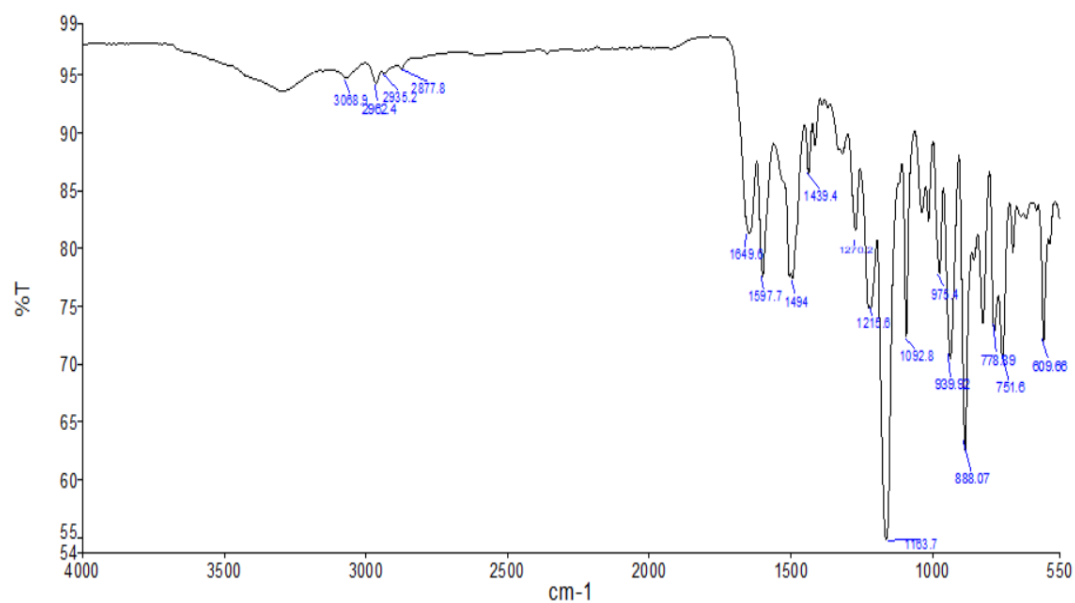


Figure S43. FT-IR (ATR) spectra of *DPP-Bnz-Val-click-4-F-Chalcone (BVK2)*

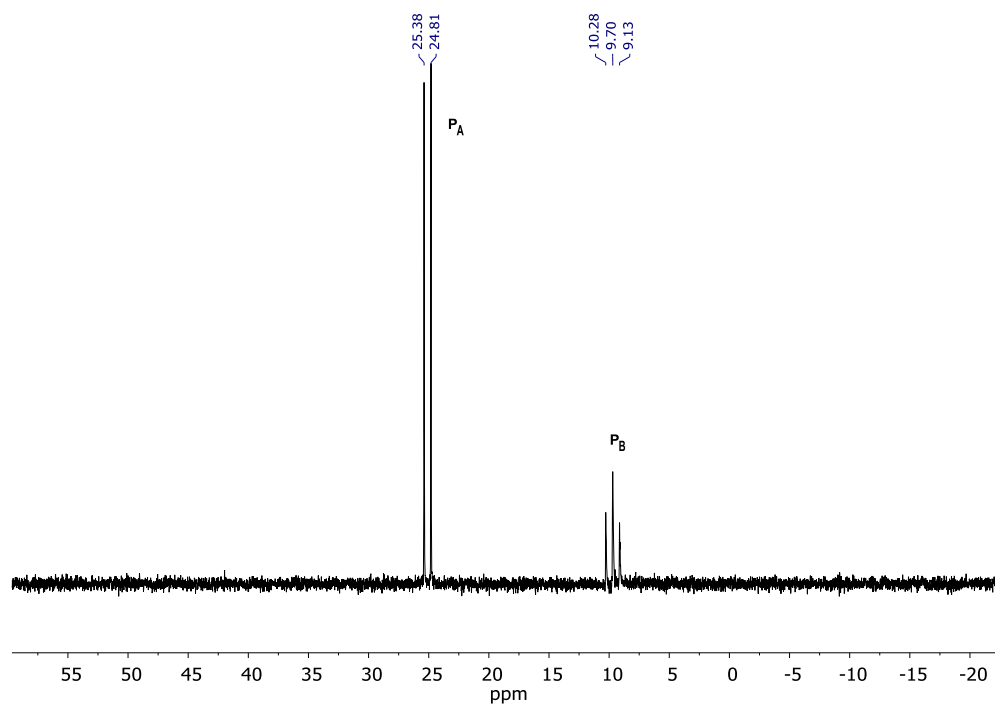


Figure S44. ^{31}P -NMR spectra of *DPP-Bnz-Val-click-4-F-Chalcone (BVK2)*

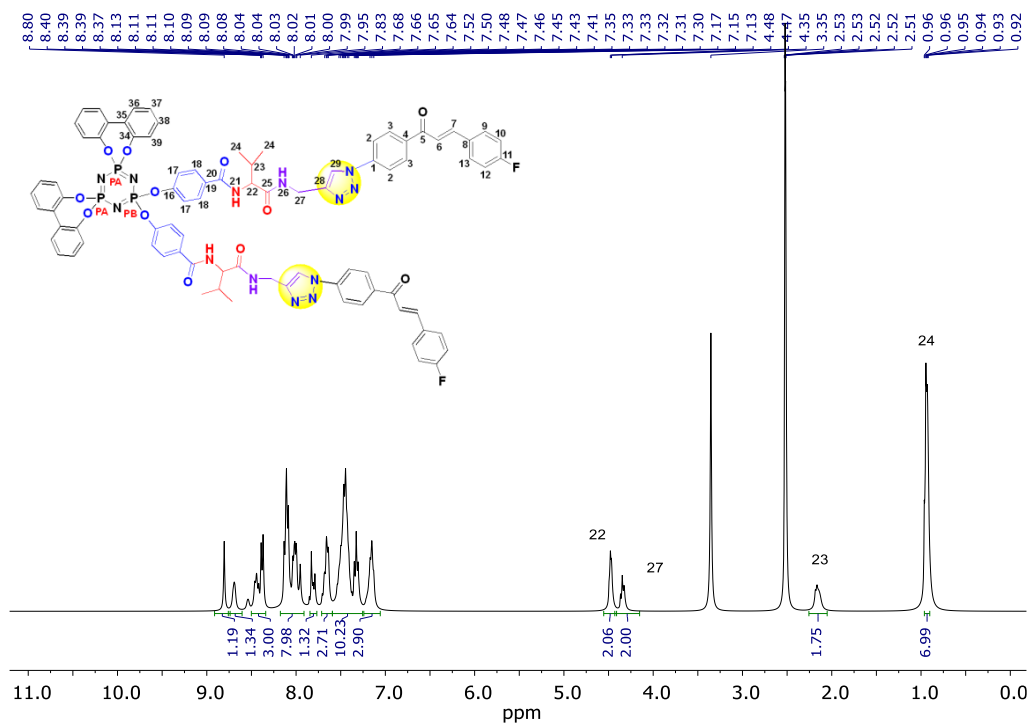


Figure S45. ^1H -NMR spectra of *DPP-Bnz-Val-click-4-F-Chalcone (BVK2)*

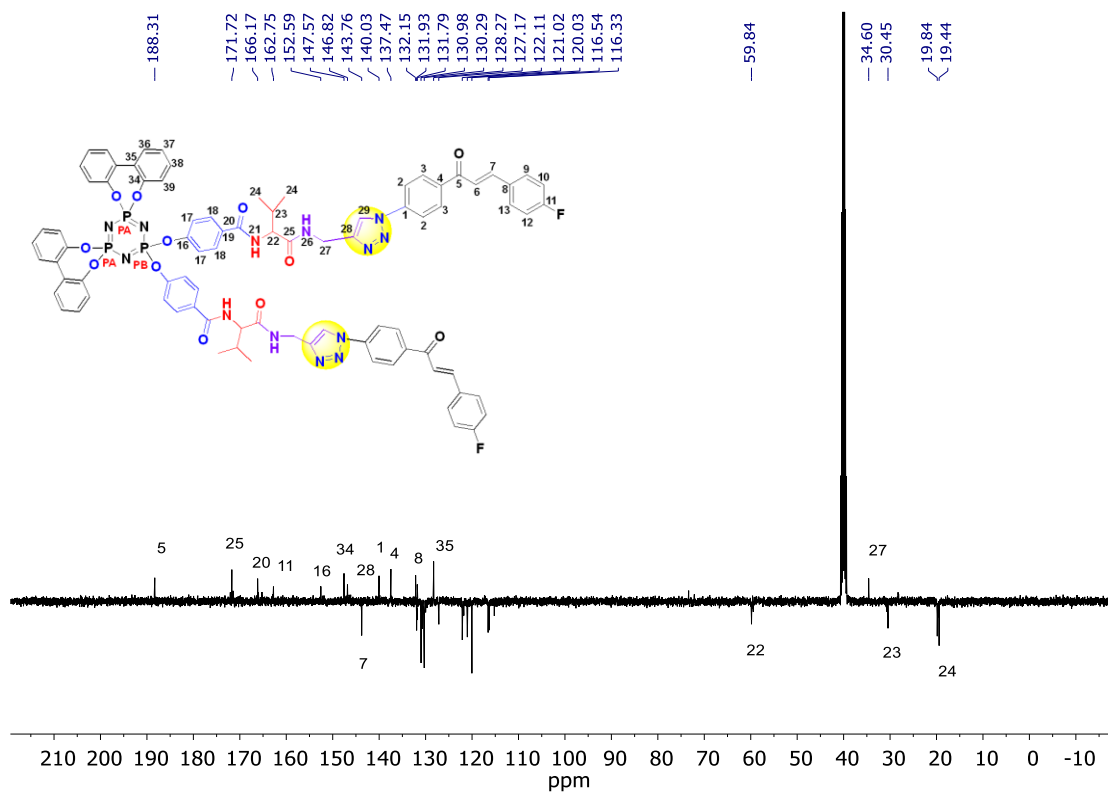


Figure S46. ^{13}C -NMR spectra of *DPP-Bnz-Val-click-4-F-Chalcone (BVK2)*

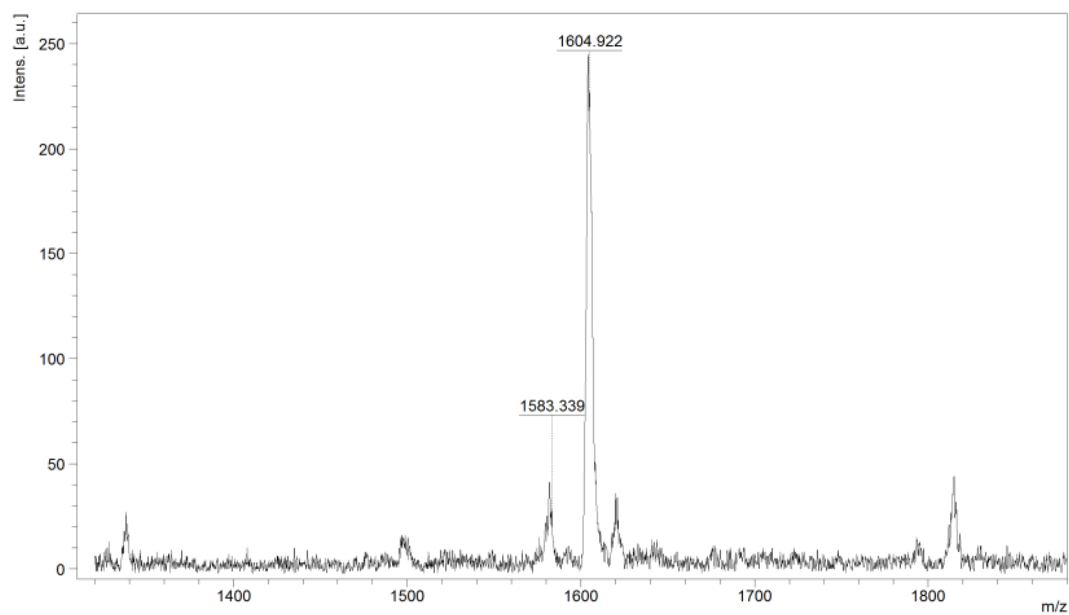


Figure S47. MALDI-TOF MS spectra of *DPP-Bnz-Val-click-4-F-Chalcone (BVK2)*

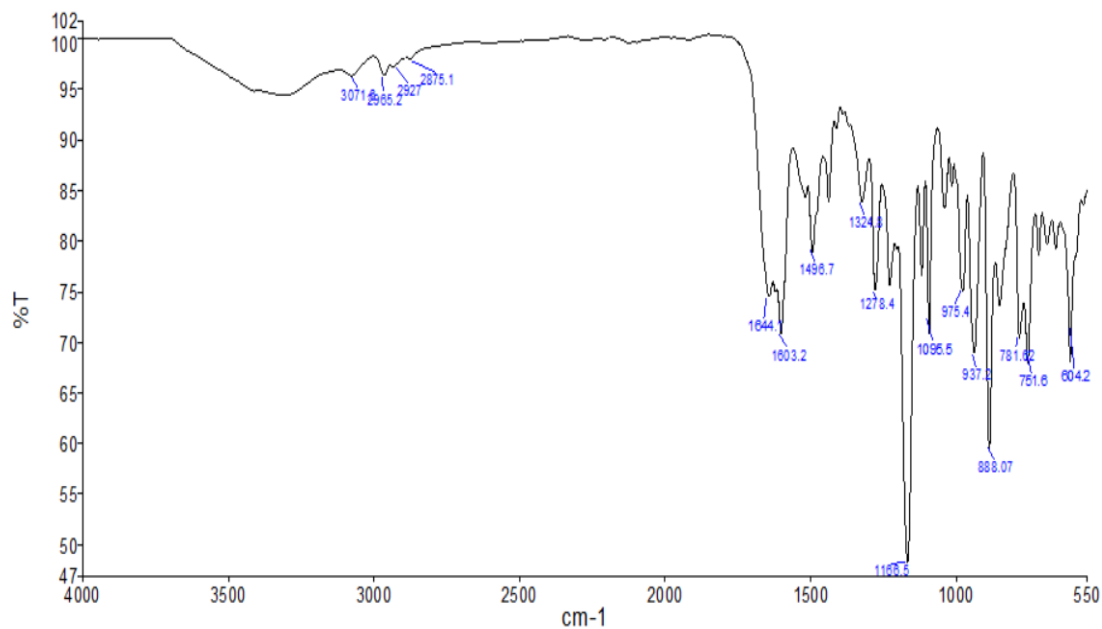


Figure S48. FT-IR (ATR) spectra of *DPP-Bnz-Val-click-3,5-difluoro-chalcone (BVK3)* (ATR)

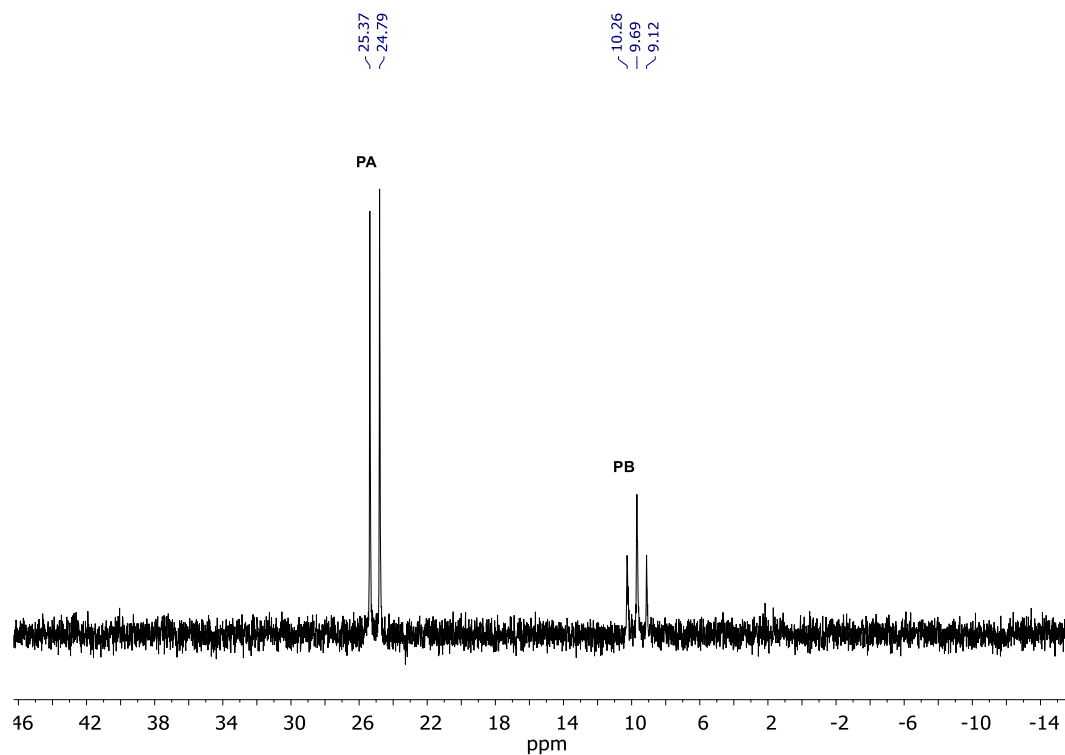


Figure S49. ³¹P-NMR spectra of *DPP-Bnz-Val-click-3,5-difluoro-chalcone (BVK3)*

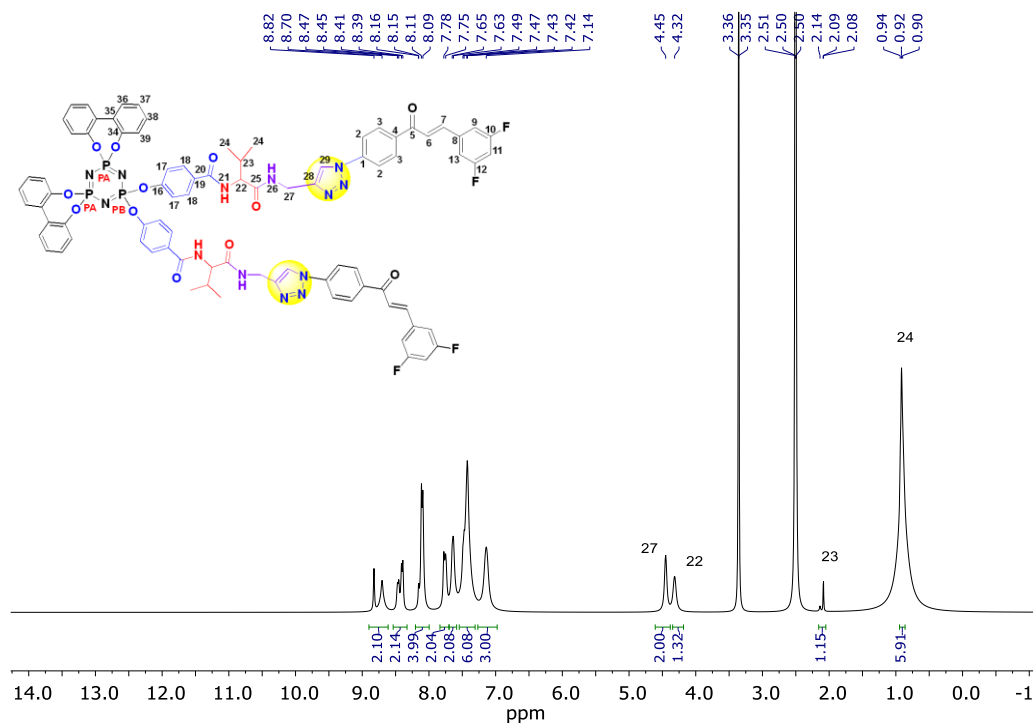


Figure S50. ¹H-NMR spectra of *DPP-Bnz-Val-click-3,5-difluoro-chalcone (BVK3)*

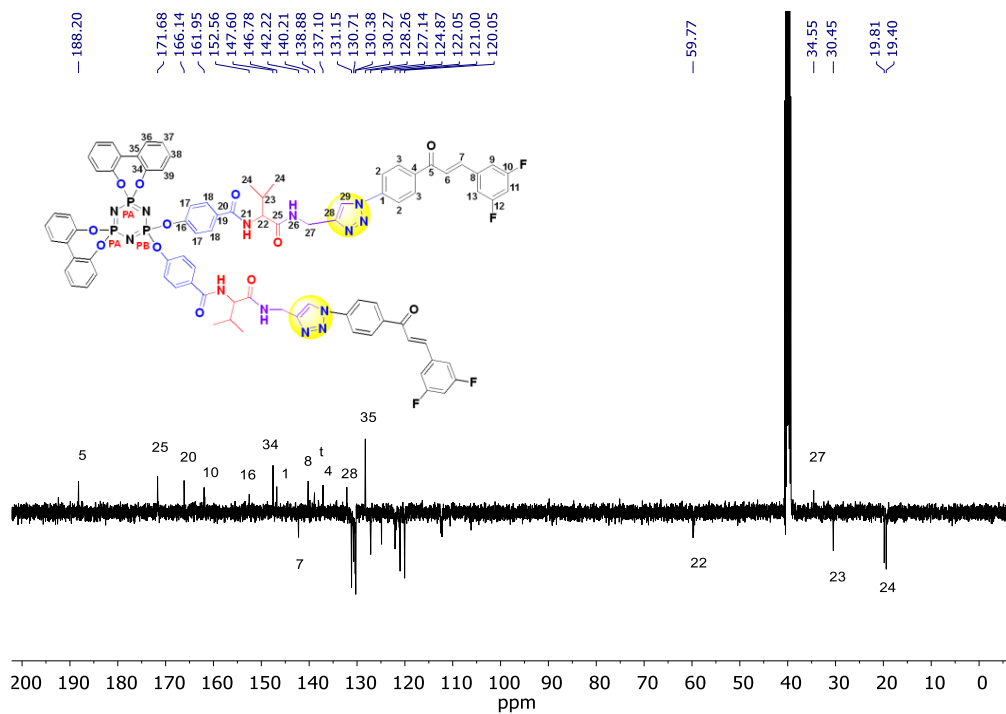


Figure S51. ¹³C-NMR spectra of *DPP-Bnz-Val-click-3,5-difluoro-chalcone (BVK3)*

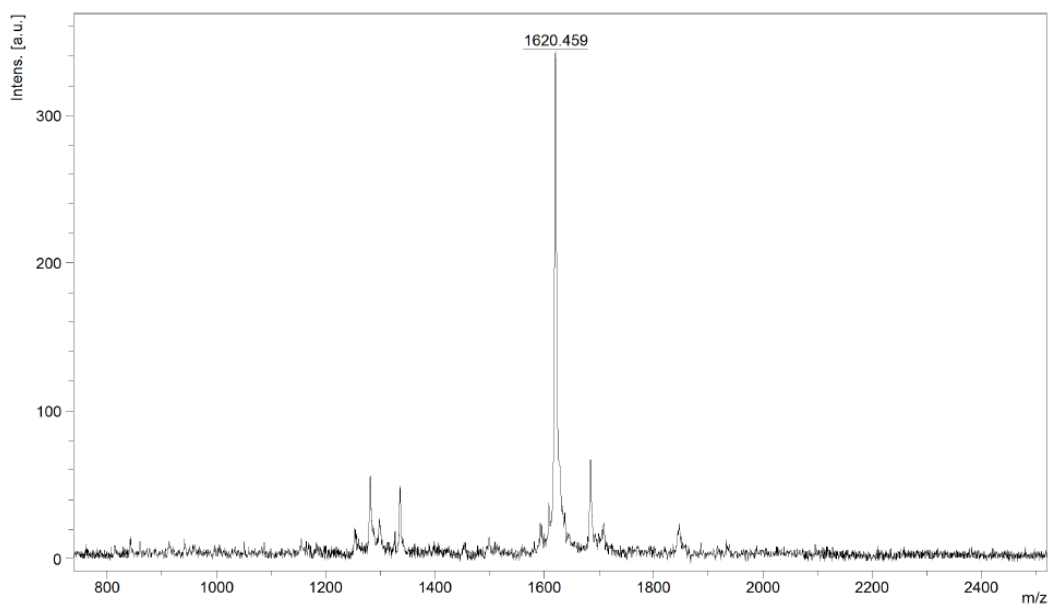


Figure S52. MALDI-TOF MS spectra of *DPP-Bnz-Val-click-3,5-difluoro-chalcone (BVK3)*

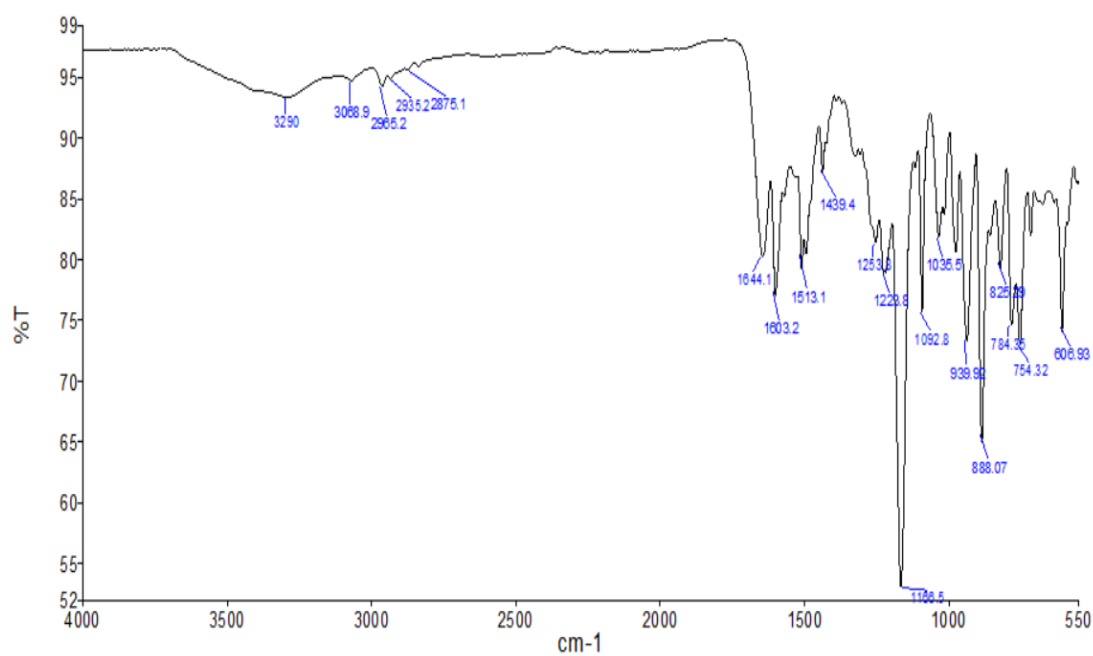


Figure S53. FT-IR (ATR) spectra of *DPP-Bnz-Val-click-4-OCH₃-chalcone (BVK4)*

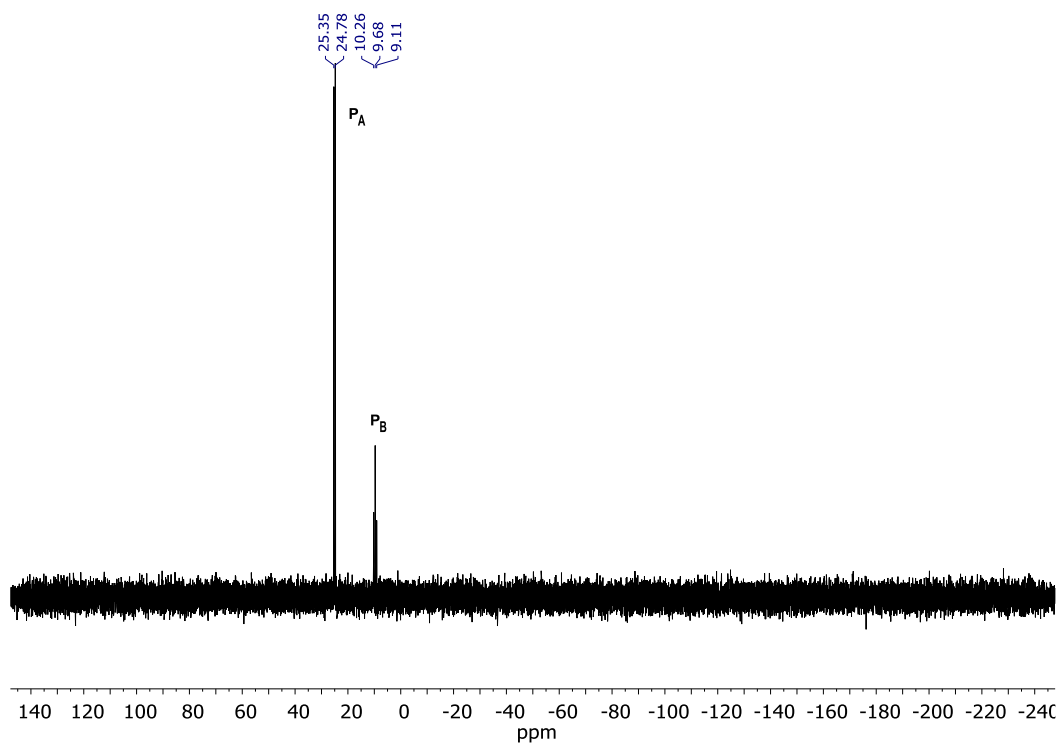


Figure S54. ³¹P-NMR spectra of *DPP-Bnz-Val-click-4-OCH₃-chalcone (BVK4)*

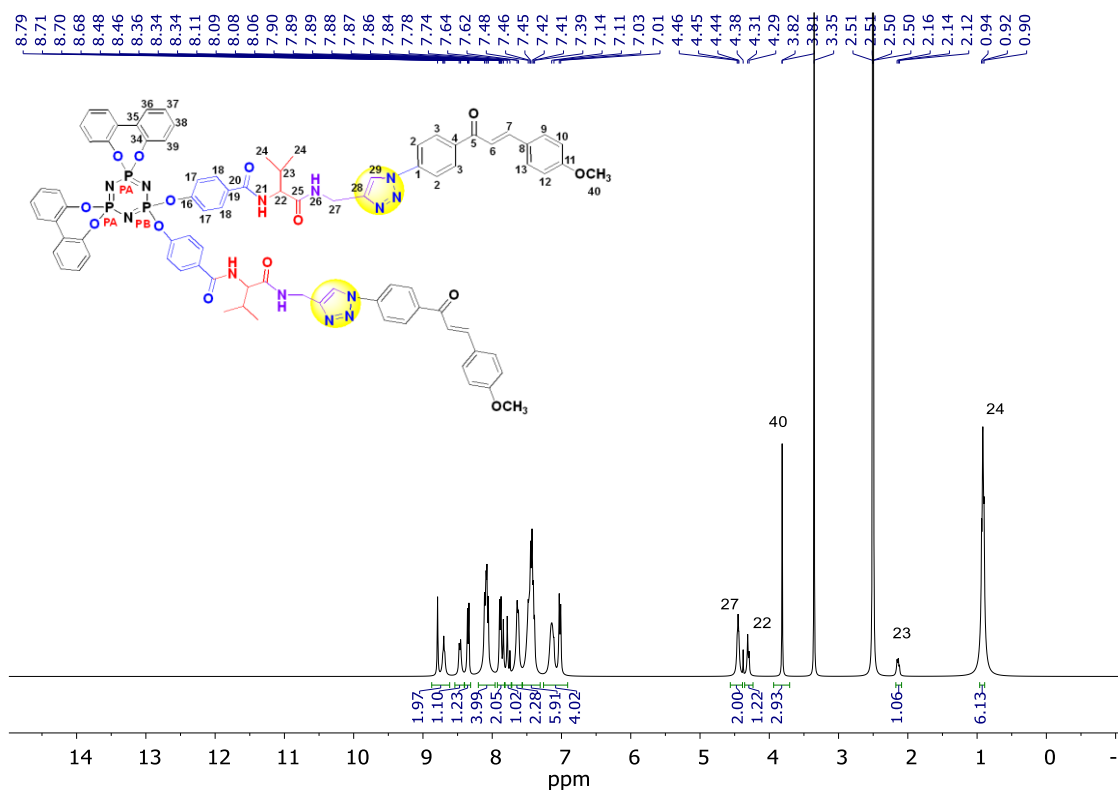


Figure S55. ¹H-NMR spectra of *DPP-Bnz-Val-click-4-OCH₃-chalcone (BVK4)*

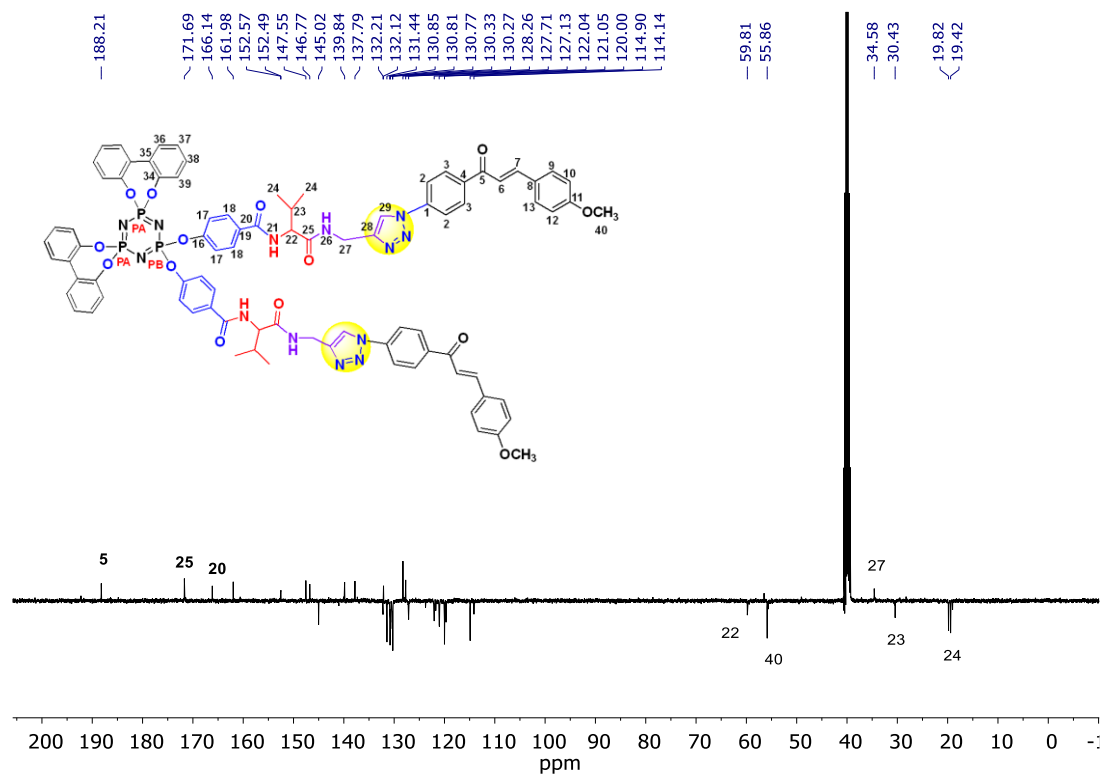


Figure S56. ¹³C-NMR spectra of *DPP-Bnz-Val-click-4-OCH₃-chalcone (BVK4)*

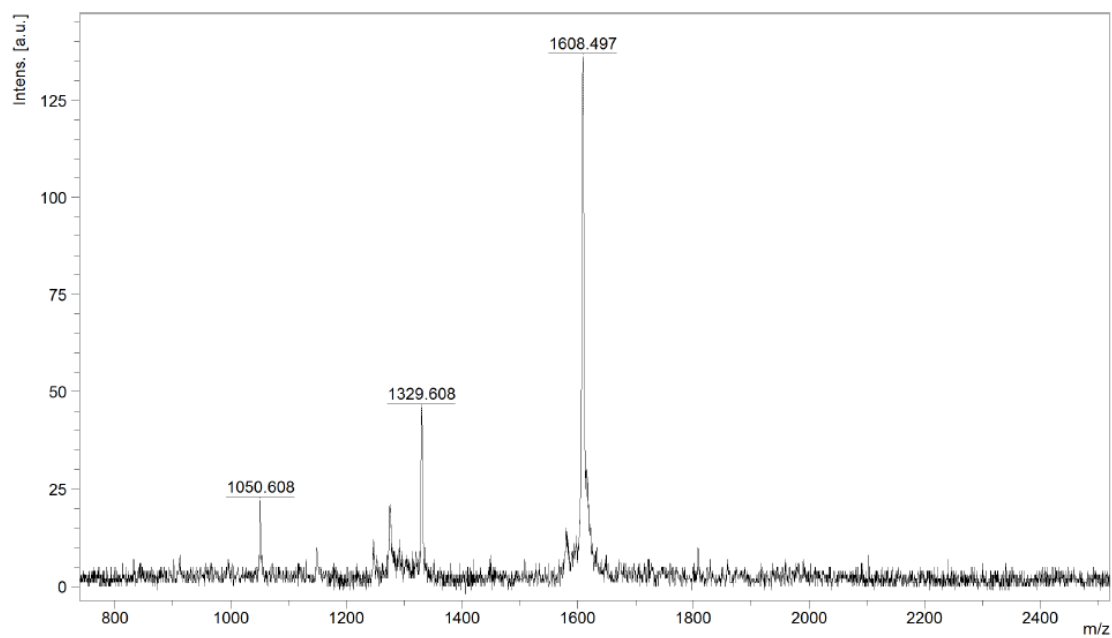


Figure S57. MALDI-TOF MS spectra of *DPP-Bnz-Val-click-4-OCH₃-chalcone (BVK4)*

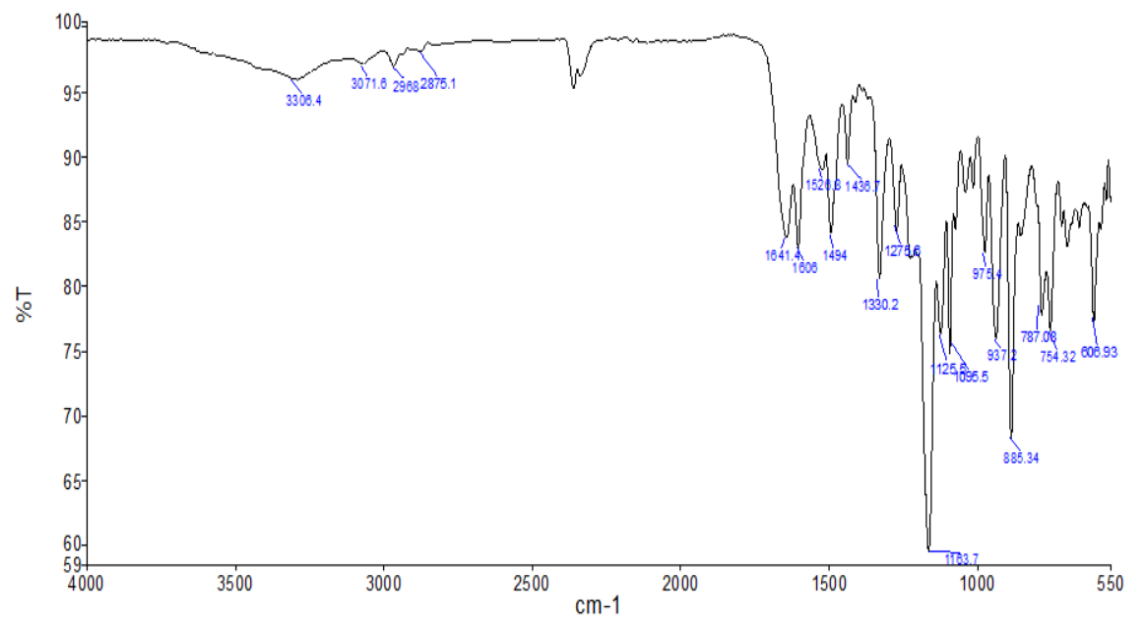


Figure S58. FT-IR (ATR) spectra of *DPP-Bnz-Val-click-3-CF₃-chalcone (BVK5)*

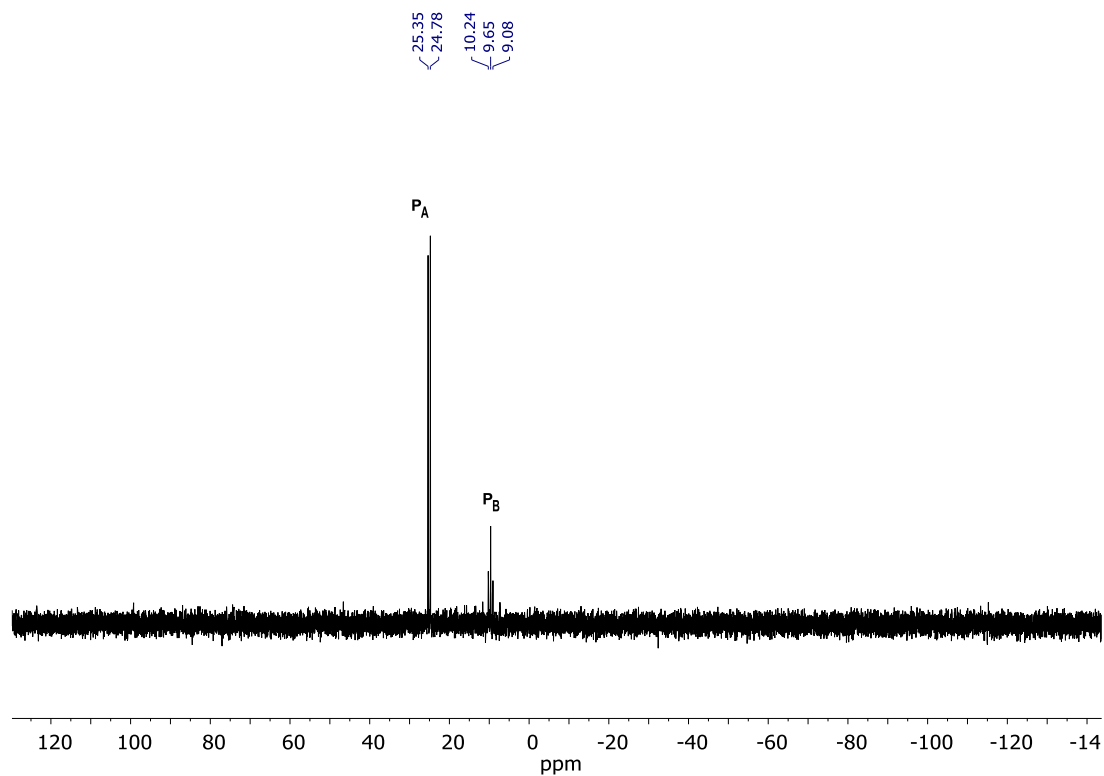


Figure S59. ³¹P-NMR spectra of *DPP-Bnz-Val-click-3-CF₃-chalcone (BVK5)*

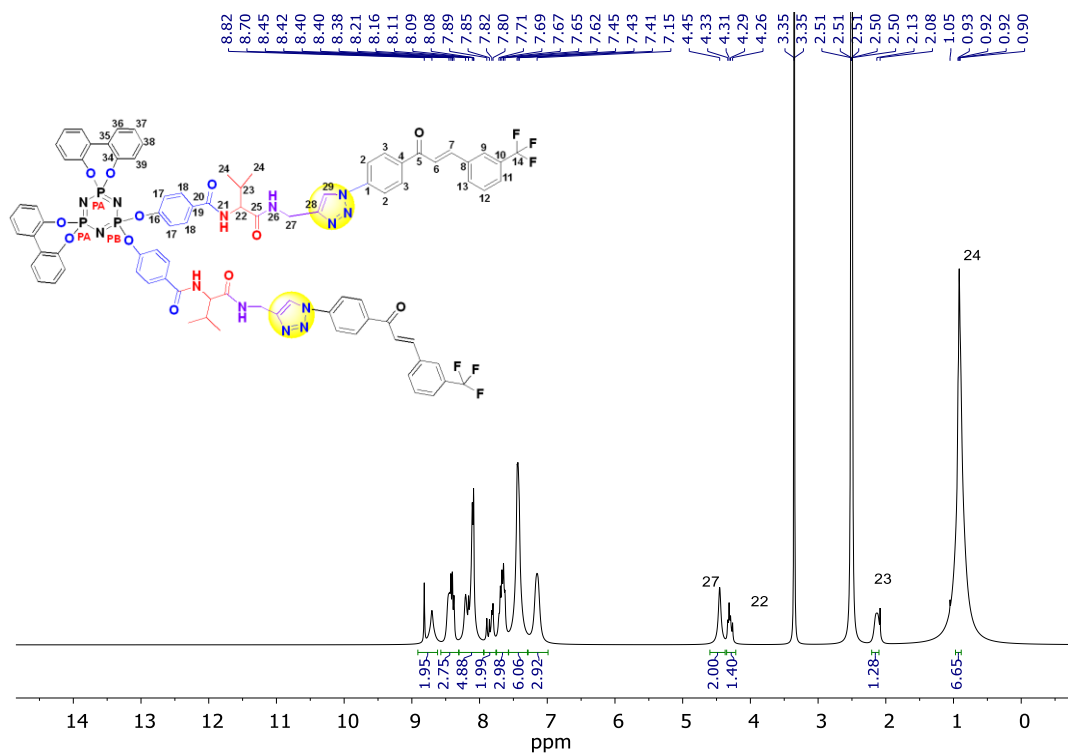


Figure S60. ¹H-NMR spectra of *DPP-Bnz-Val-click-3-CF₃-chalcone (BVK5)*

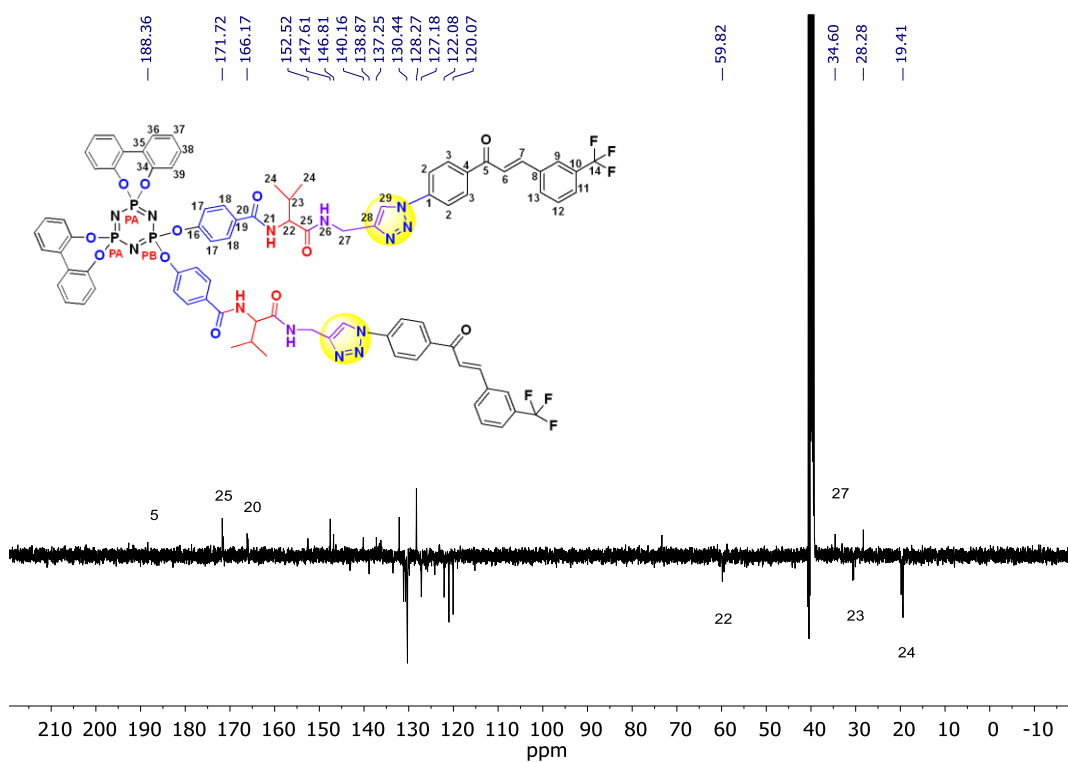


Figure S61. ¹³C-NMR spectra of *DPP-Bnz-Val-click-3-CF₃-chalcone (BVK5)*

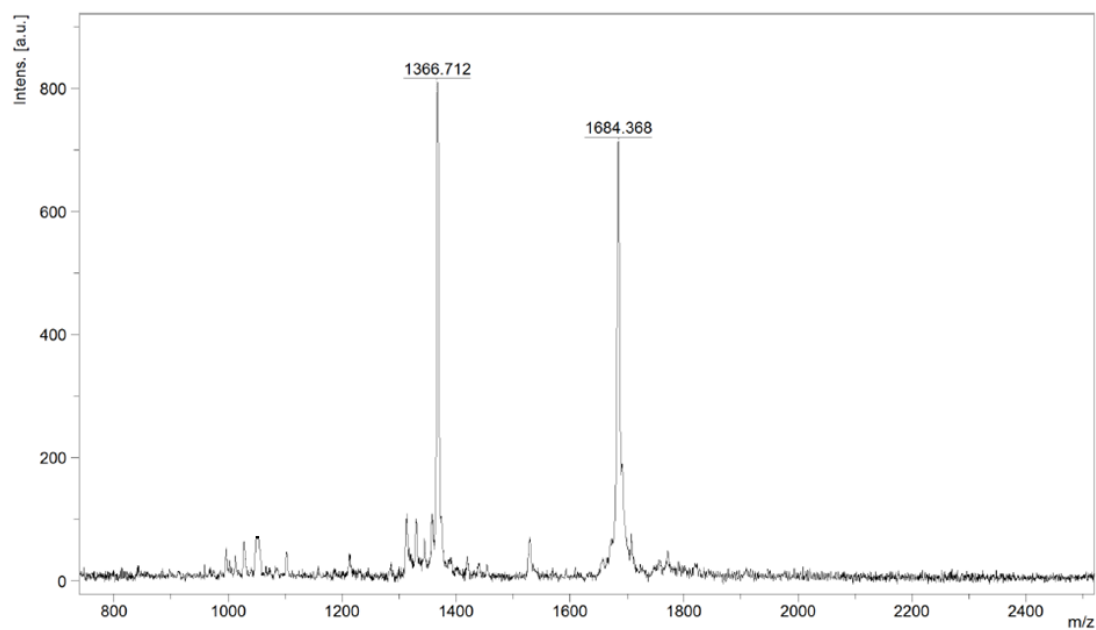


Figure S62. MALDI-TOF MS spectra of *DPP-Bnz-Val-click-3-CF₃-chalcone (BVK5)*

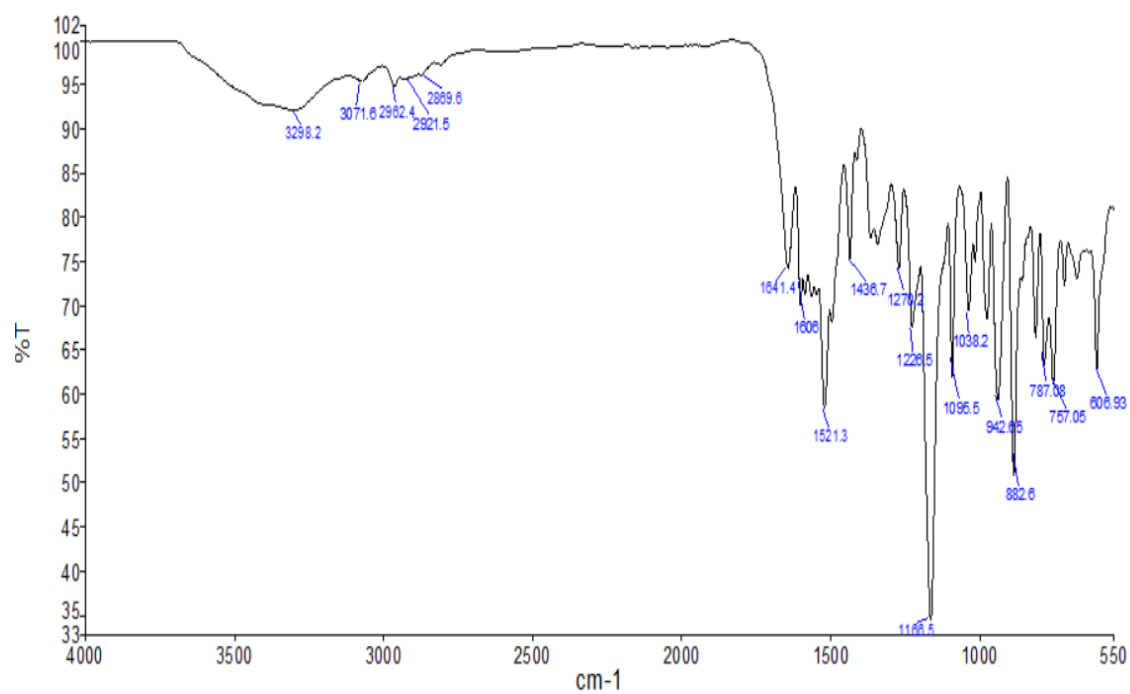


Figure S63. FT-IR (ATR) spectra of *DPP-Bnz-Val-click-4-N(CH₃)₂-chalcone (BVK6)*

