

Supplementary Information

Synthesis and photophysical properties of aromatic L-amino acids
functionalized tricyanofuran (TCF) derivatives

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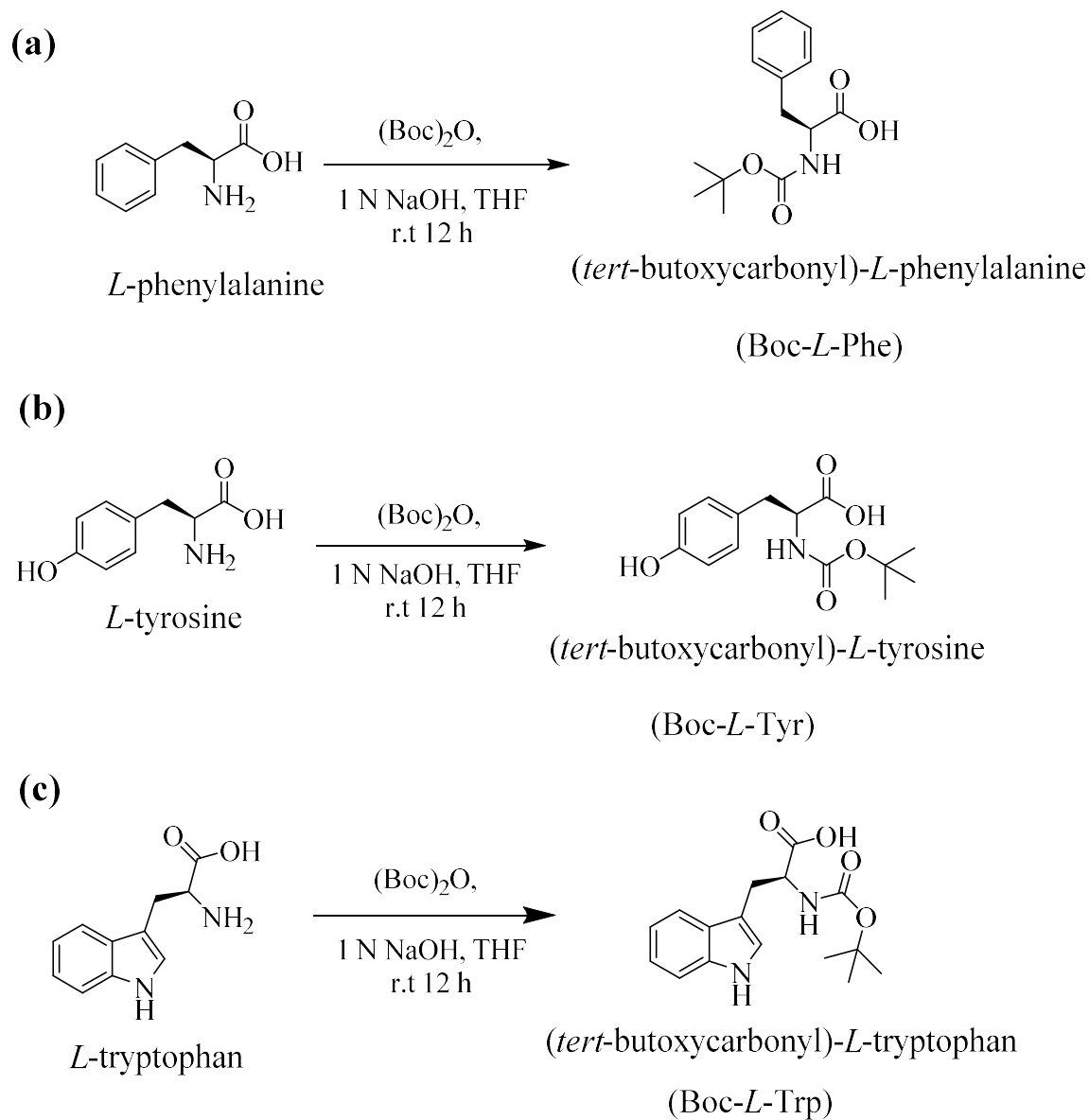
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Scheme 1. Synthetic route for Boc-*L*-Phe, Boc-*L*-Tyr and Boc-*L*-Trp.

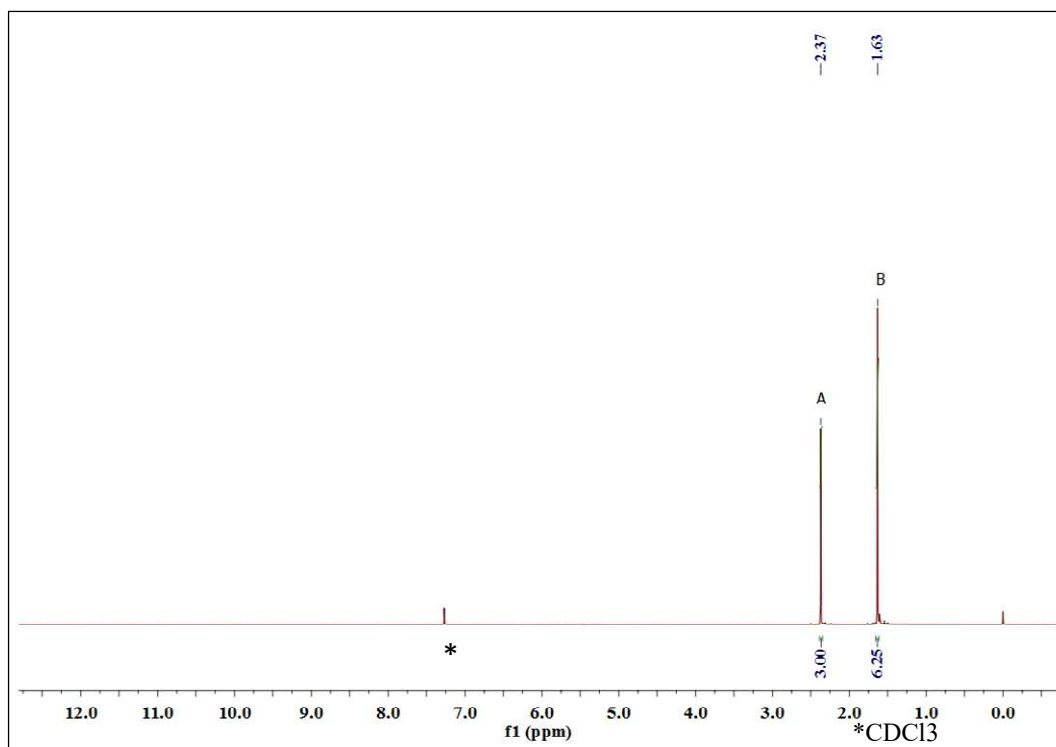


Figure S1. ^1H NMR spectra of compound 2-(3-cyano-4,5,5-trimethylfuran-2(5H)-ylidene) malonitrile (TCF) (2).

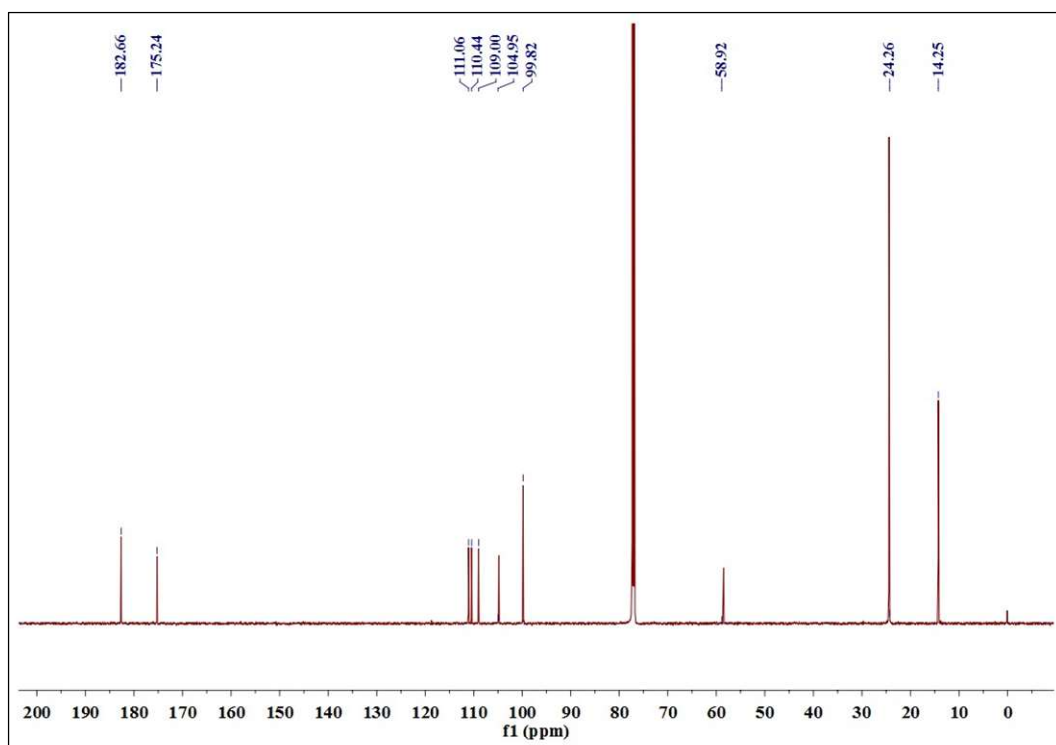


Figure S2. ^{13}C NMR spectra of compound 2-(3-cyano-4,5,5-trimethylfuran-2(5H)-ylidene) malonitrile (TCF) (2).

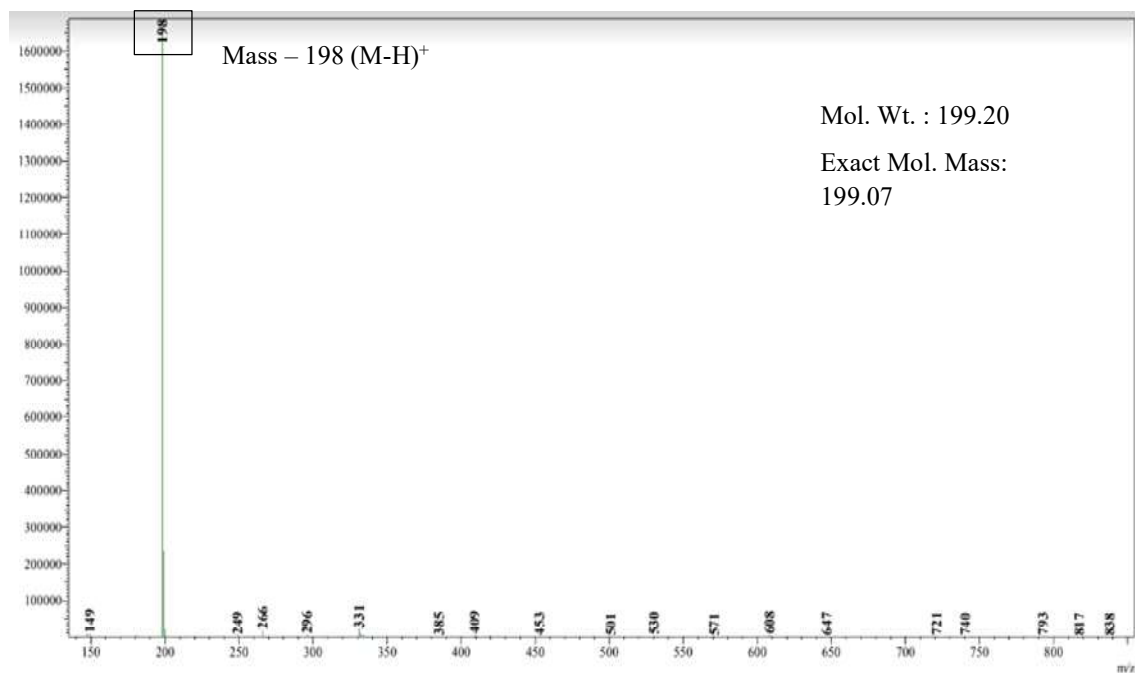


Figure S3. LCMS spectrum of compound 2-(3-cyano-4,5,5-trimethylfuran-2(5H)-ylidene) malonitrile (TCF) (2).

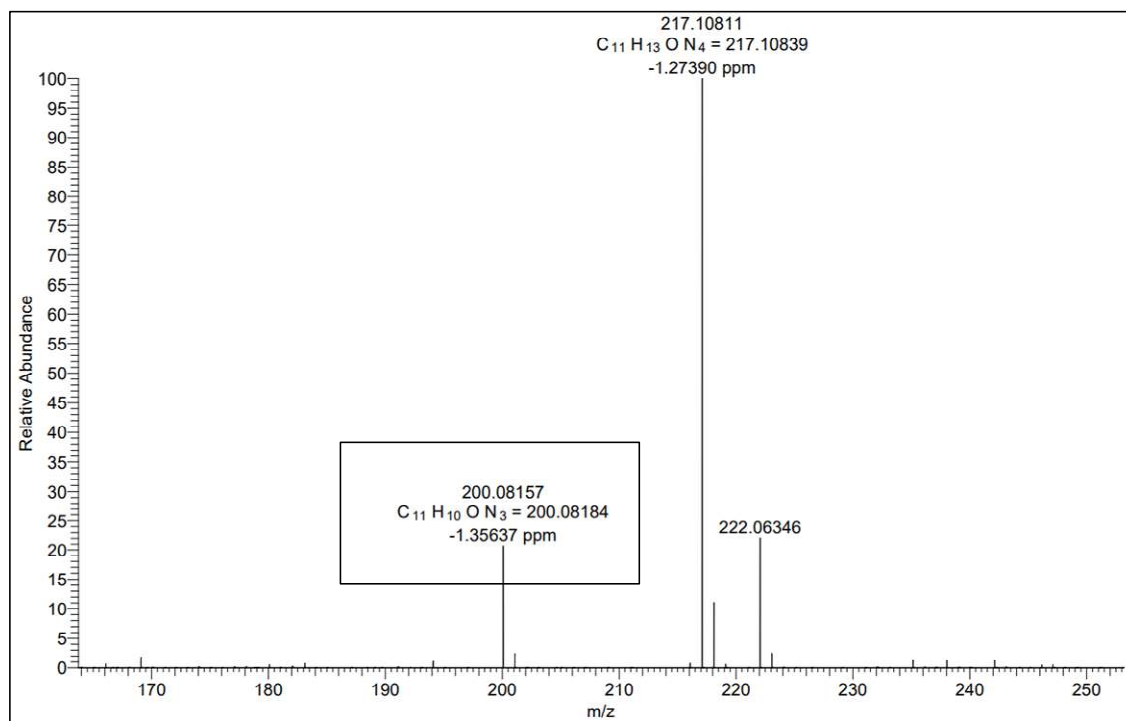


Figure S4. HRMS spectrum of compound 2-(3-cyano-4,5,5-trimethylfuran-2(5H)-ylidene) malonitrile (TCF) (2).

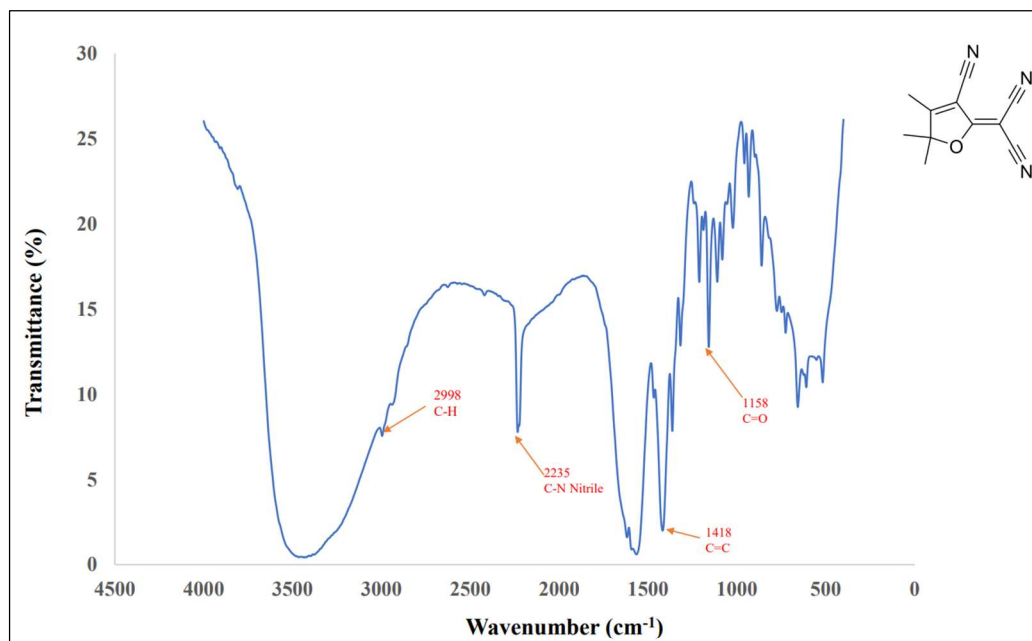


Figure S5. FT-IR spectra of compound 2-(3-cyano-4,5,5-trimethylfuran-2(5H)-ylidene) malononitrile (TCF) (2).

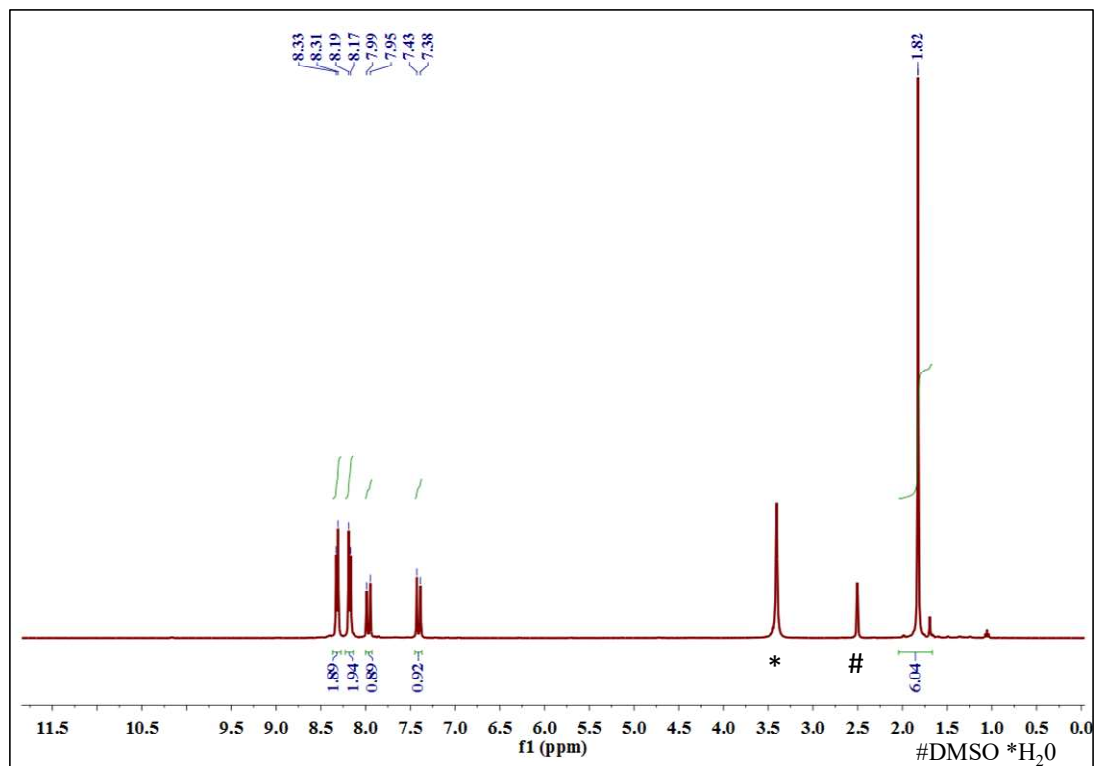


Figure S6. ¹H NMR spectra of compound (*E*)-2-(3-cyano-5,5-dimethyl-4-(4-nitrostyryl) furan-2(5H) ylidene) malononitrile (3).

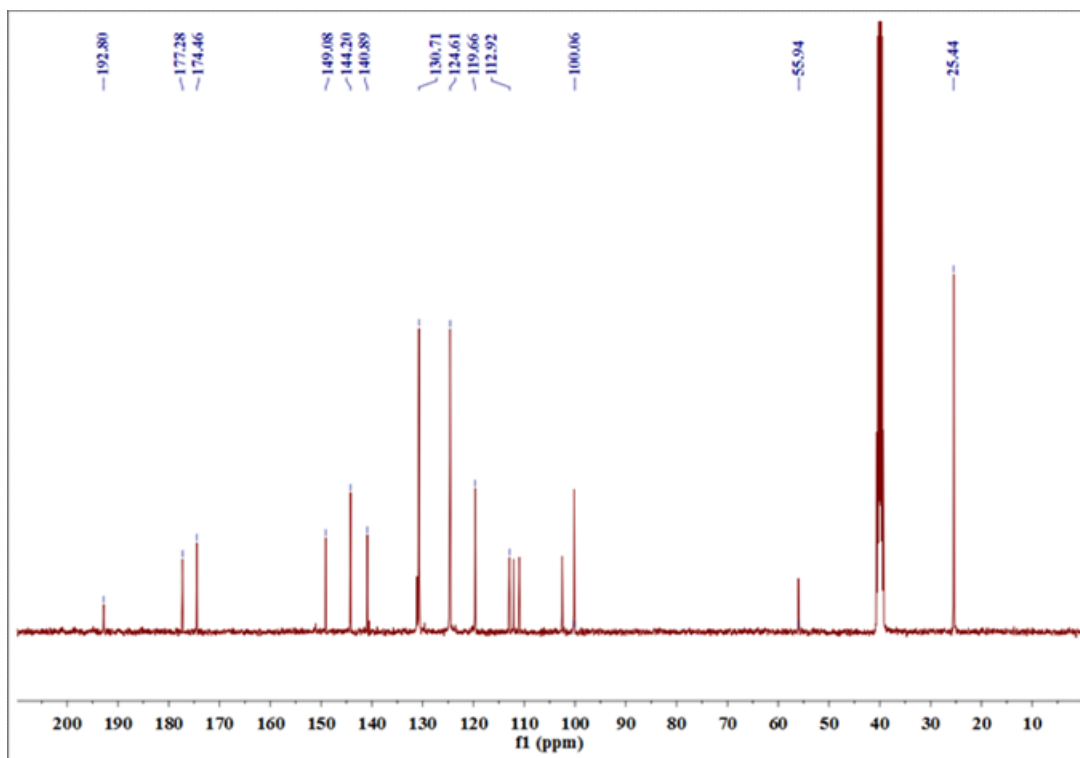


Figure S7. ^{13}C NMR spectra of compound (*E*)-2-(3-cyano-5,5-dimethyl-4-(4-nitrostyryl) furan-2(5H) ylidene) malononitrile (3).

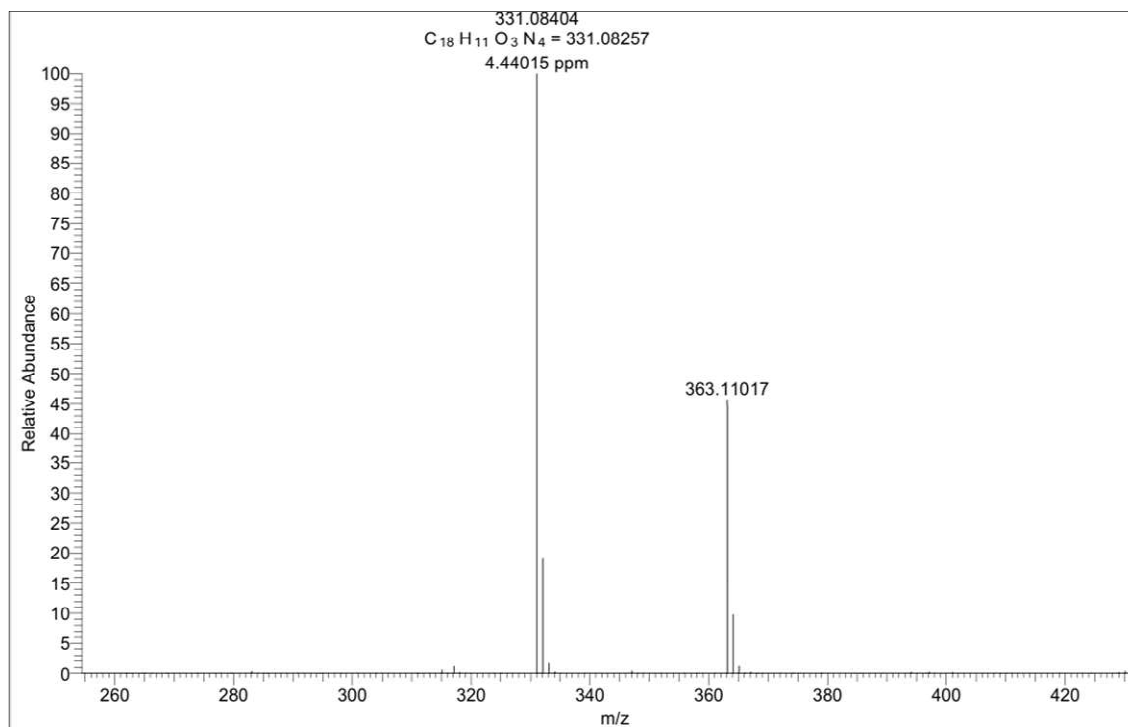


Figure S8. HRMS spectrum of compound (*E*)-2-(3-cyano-5,5-dimethyl-4-(4-nitrostyryl) furan-2(5H) ylidene) malononitrile (3).

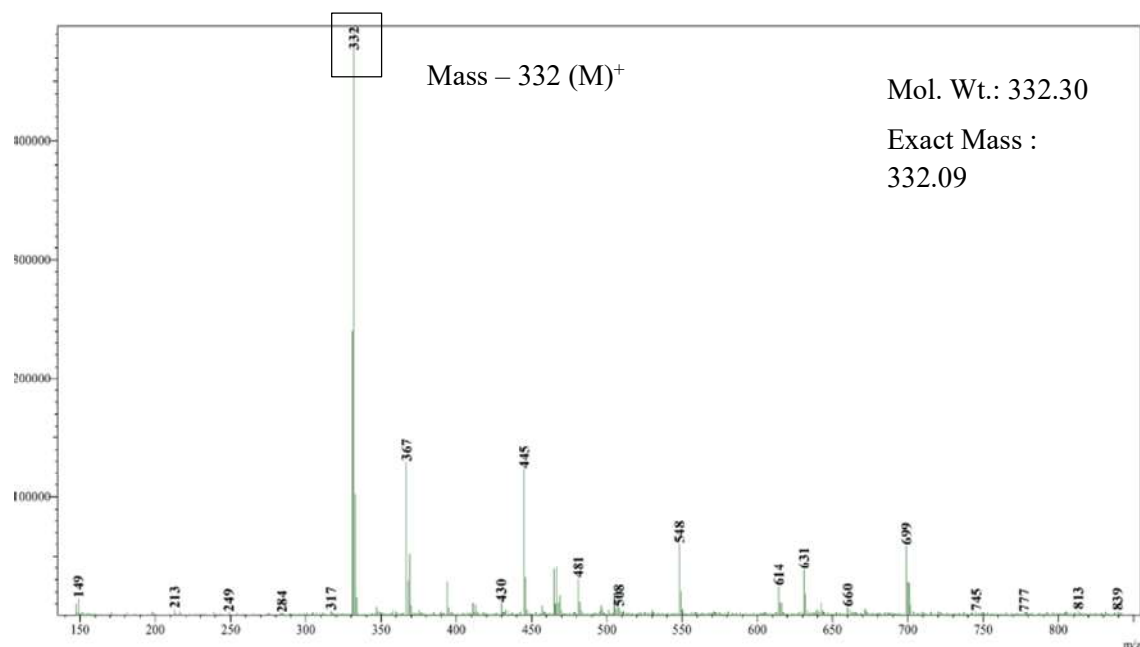


Figure S9. LCMS spectrum of compound (*E*)-2-(3-cyano-5,5-dimethyl-4-(4-nitrostyryl) furan-2(5H) ylidene) malononitrile (3).

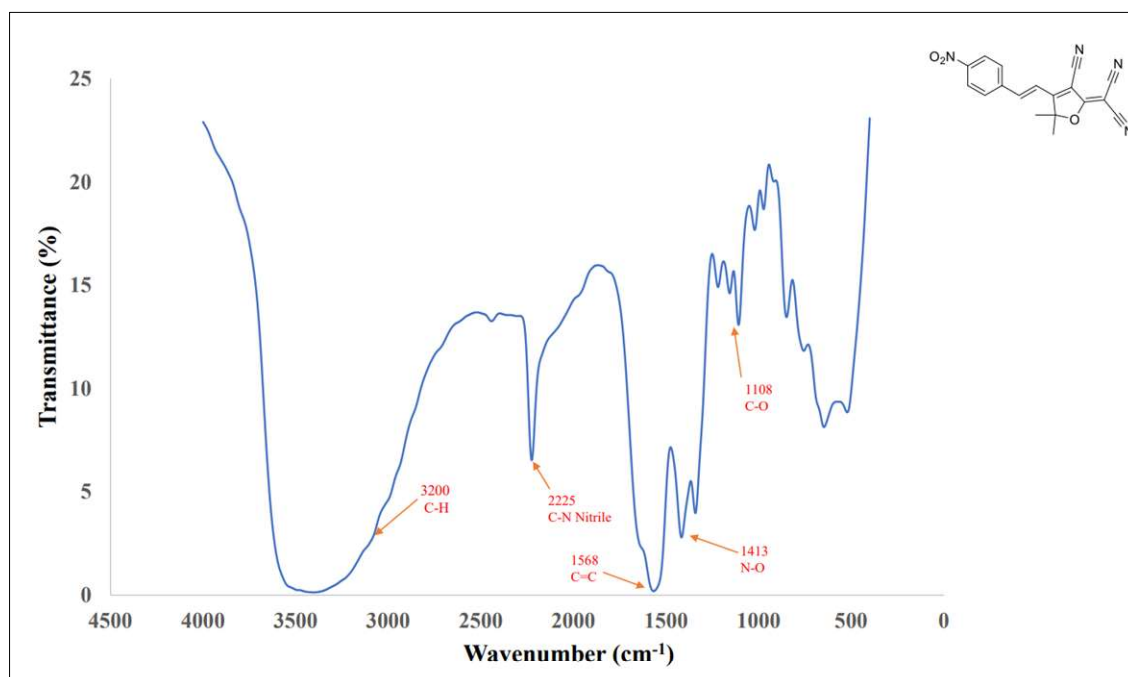


Figure S10. FT-IR spectra of compound (*E*)-2-(3-cyano-5,5-dimethyl-4-(4-nitrostyryl) furan-2(5H) ylidene) malononitrile (3).

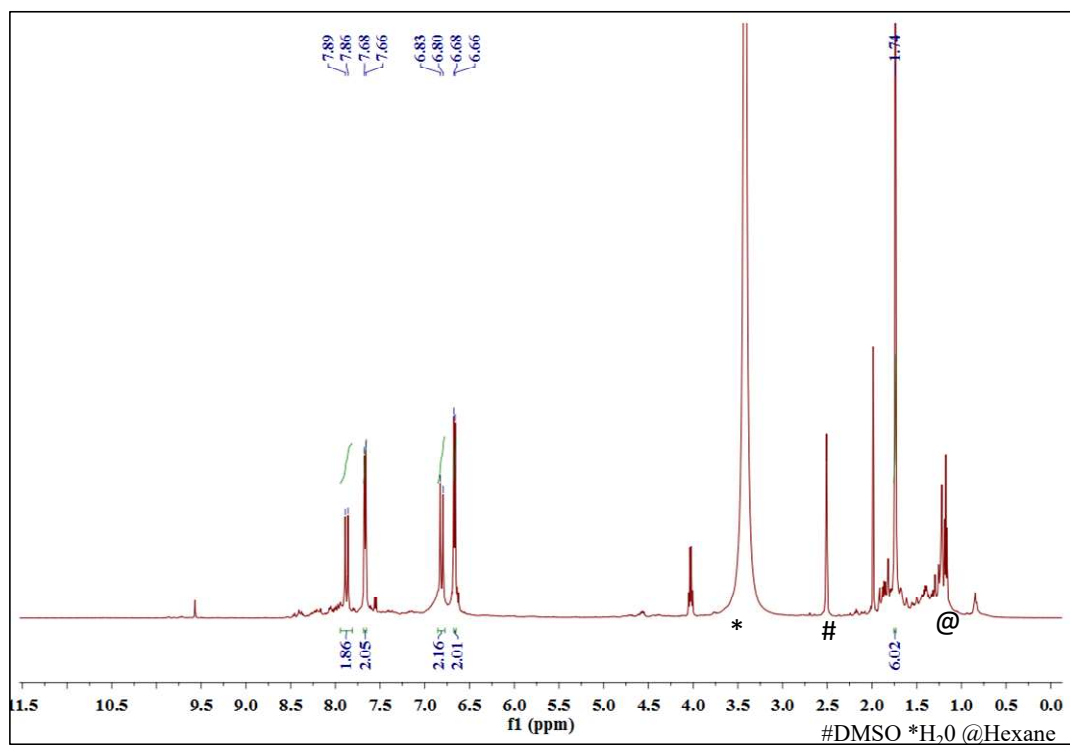


Figure S11. ¹H NMR spectra of compound (*E*)-2-(4-(4-aminostyryl)-3-cyano-5,5-dimethylfuran-2(5H) ylidene) malononitrile as TCF-1 (4).

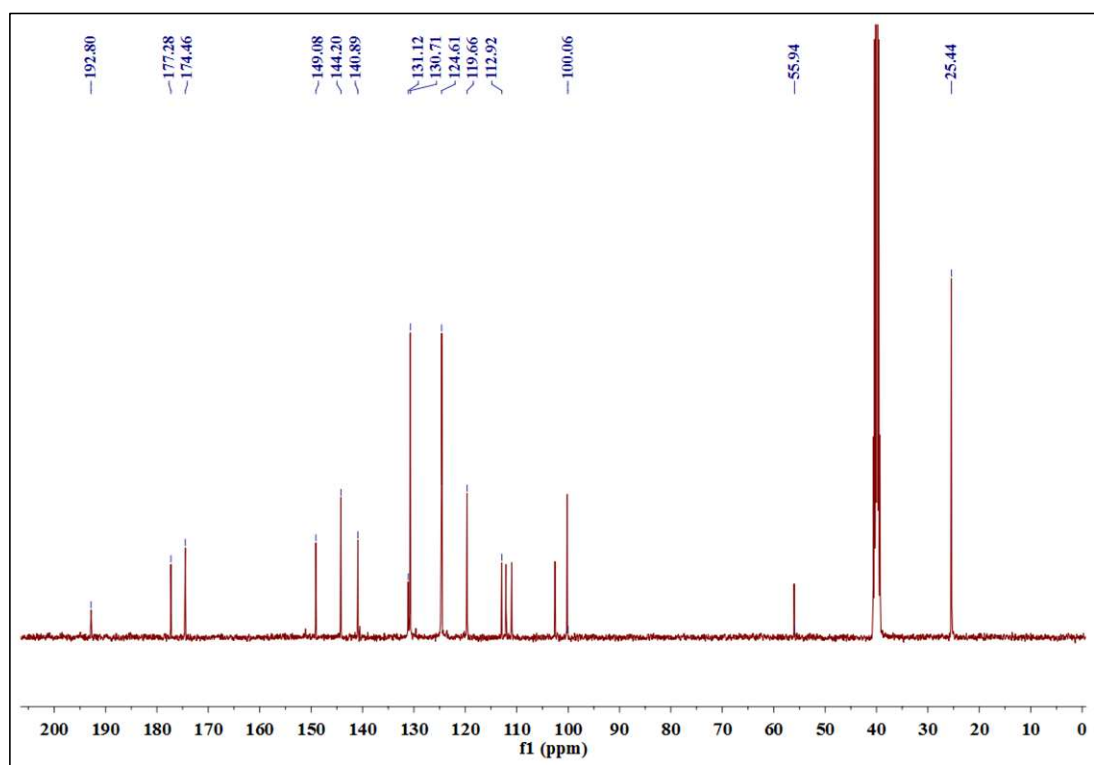


Figure S12. ¹³C NMR spectra of compound (*E*)-2-(4-(4-aminostyryl)-3-cyano-5,5-dimethylfuran-2(5H) ylidene) malononitrile as TCF-1 (4).

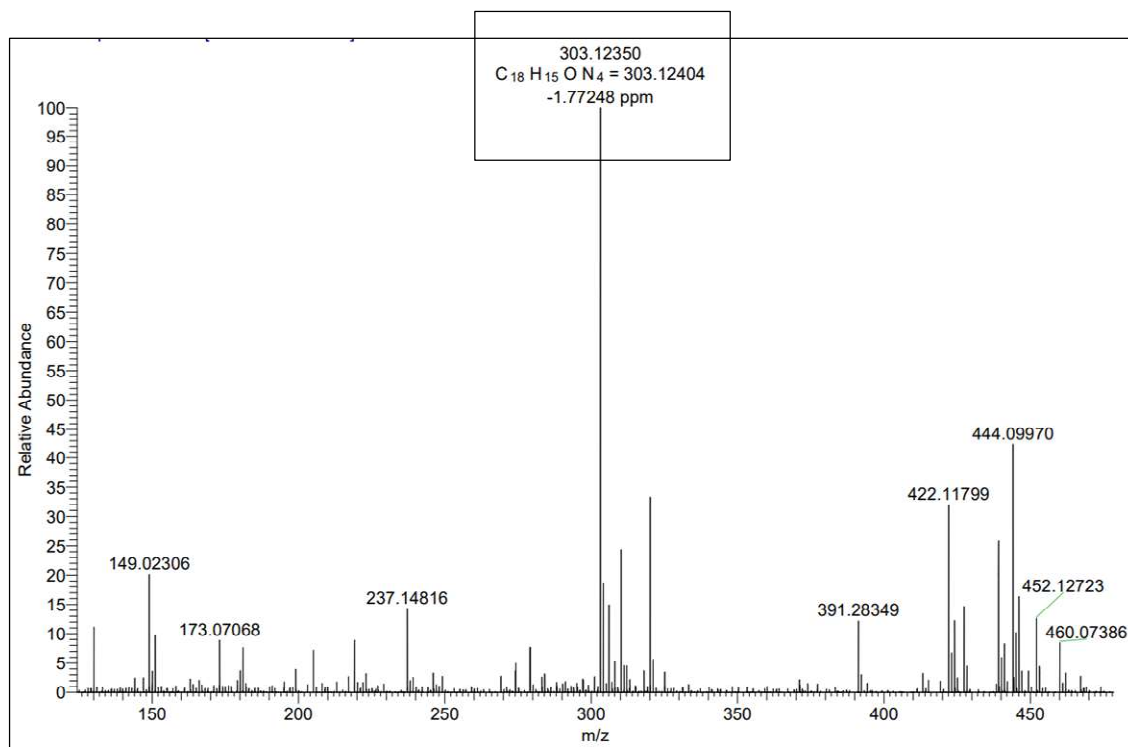


Figure S13. HRMS spectrum of compound (*E*)-2-(4-(4-aminostyryl)-3-cyano-5,5-dimethylfuran-2(5H) ylidene) malononitrile as TCF-1 (4).

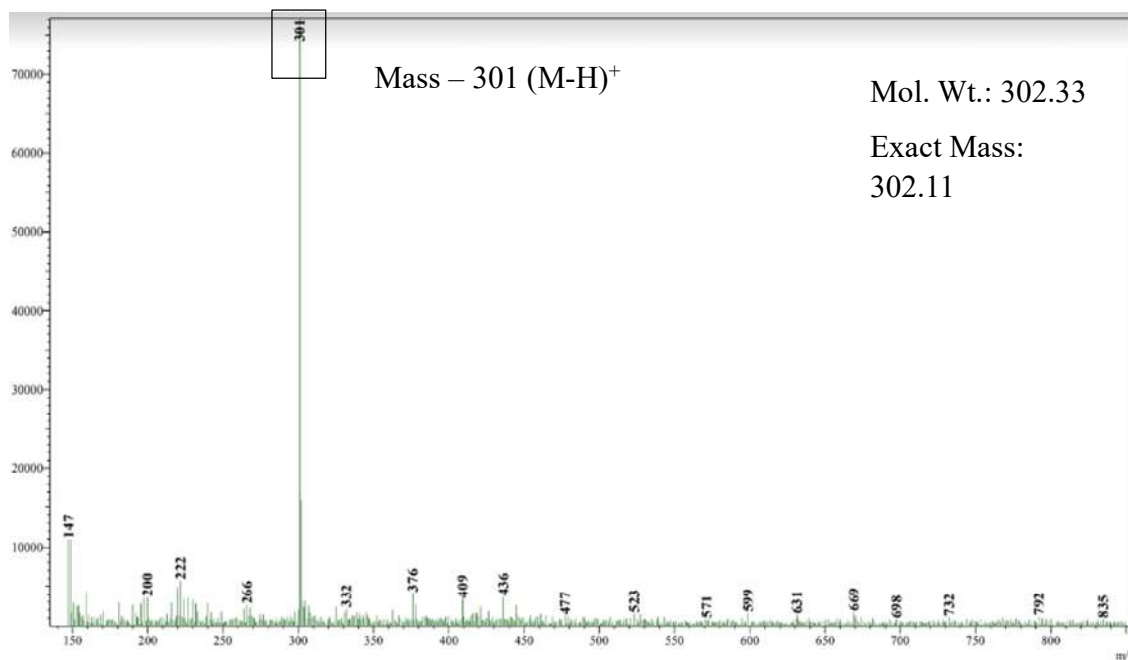


Figure S14. LCMS spectrum of compound (*E*)-2-(4-(4-aminostyryl)-3-cyano-5,5-dimethylfuran-2(5H) ylidene) malononitrile as TCF-1 (4).

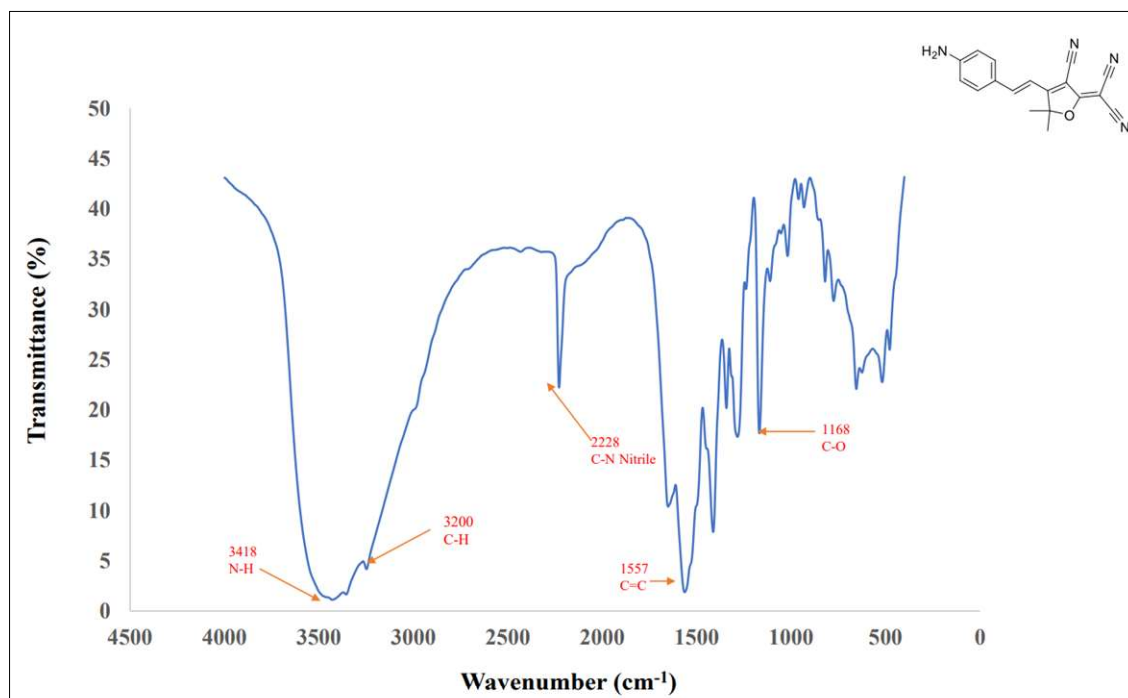


Figure S15. FT-IR spectra of compound (E)-2-(4-(4-aminostyryl)-3-cyano-5,5-dimethylfuran-2(5H) ylidene) malononitrile as TCF-1 (4).

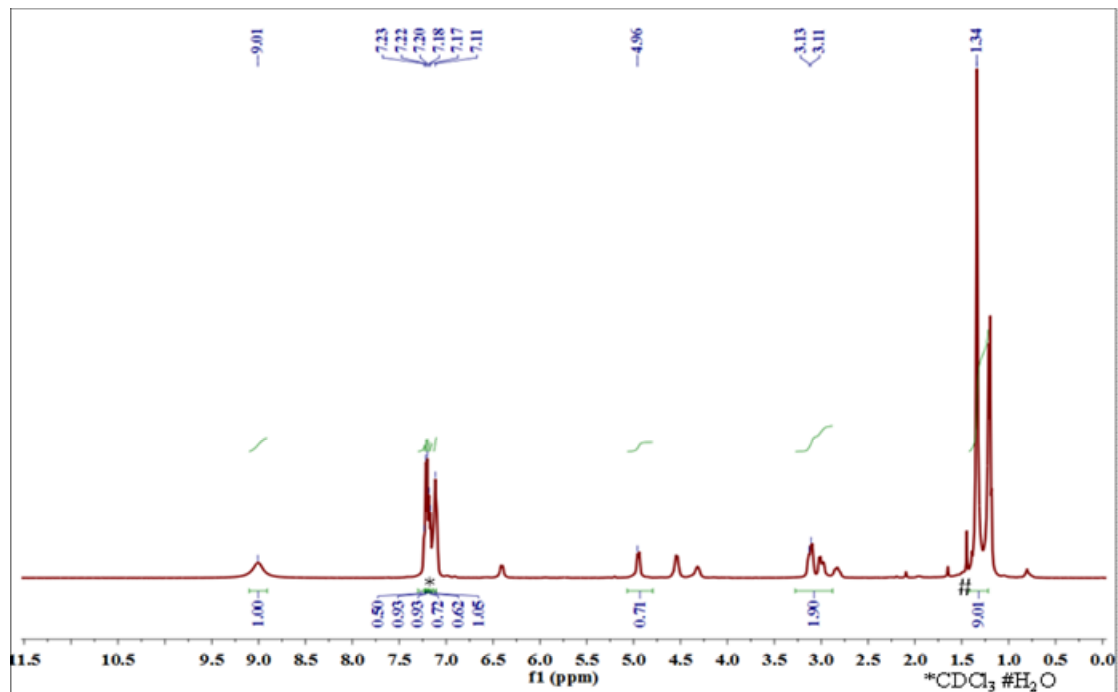


Figure S36. ¹H NMR spectra of compound (tert-butoxycarbonyl)-L-phenylalanine (Boc-L-Phe).

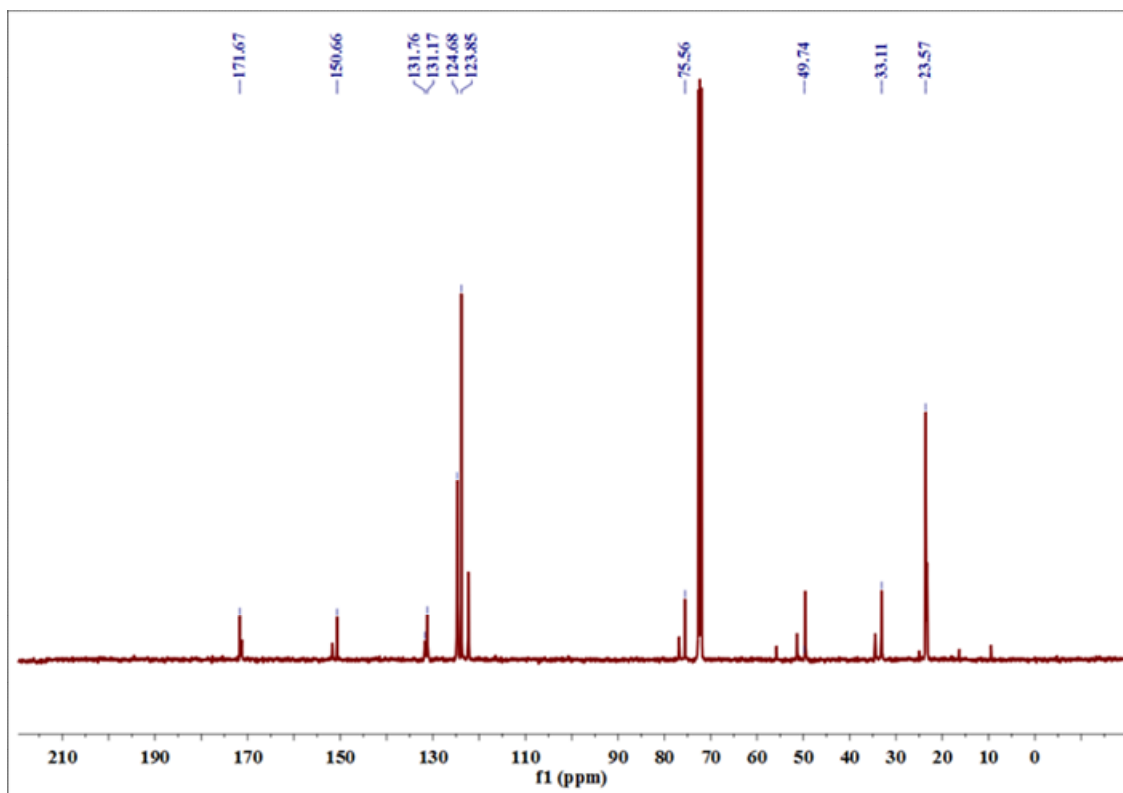


Figure S37. ^{13}C NMR spectra of compound (*tert*-butoxycarbonyl)-L-phenylalanine (Boc-*L*-Phe).

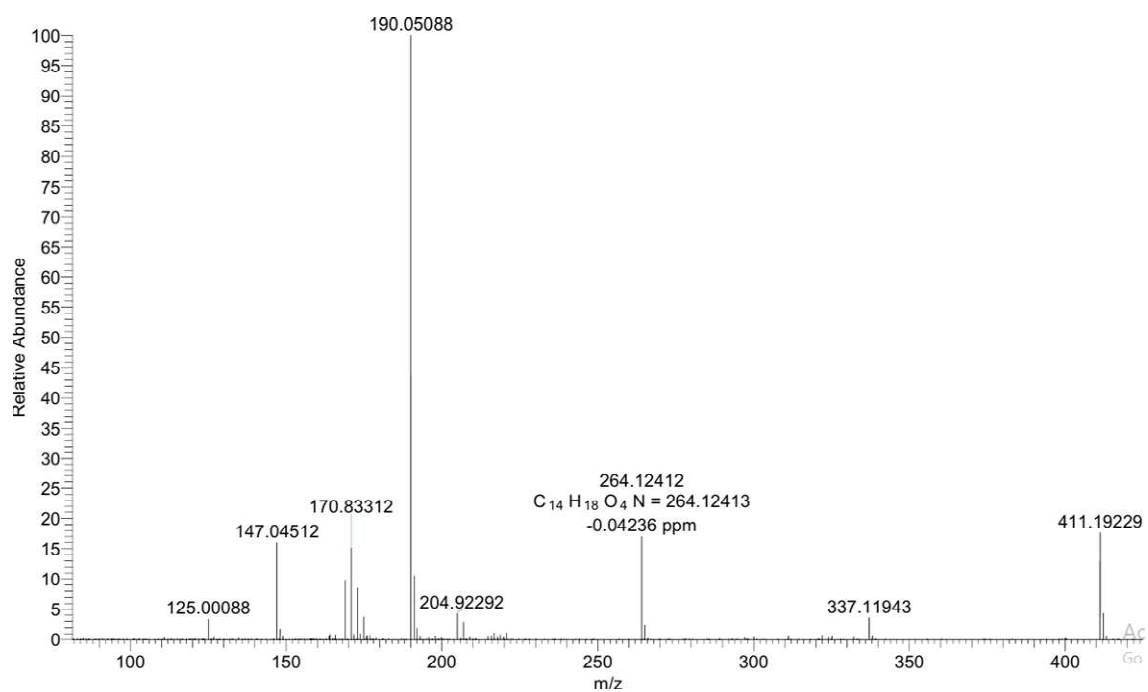


Figure S38. HRMS spectrum of compound (*tert*-butoxycarbonyl)-L-phenylalanine (Boc-*L*-Phe).

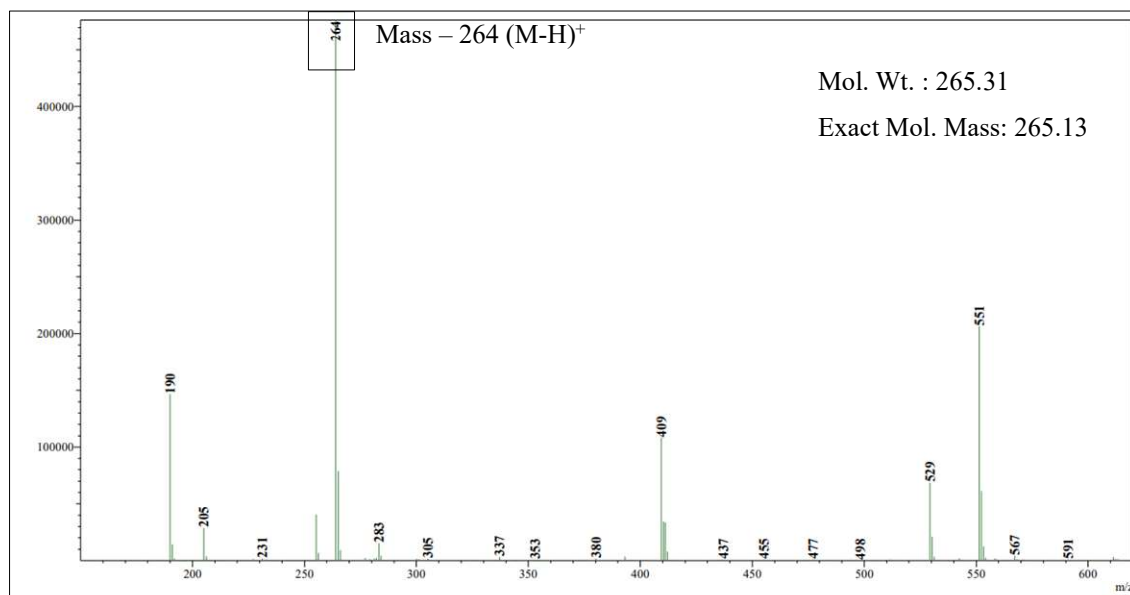


Figure S39. LCMS spectrum of compound (*tert*-butoxycarbonyl)-L-phenylalanine (Boc-*L*-Phe).

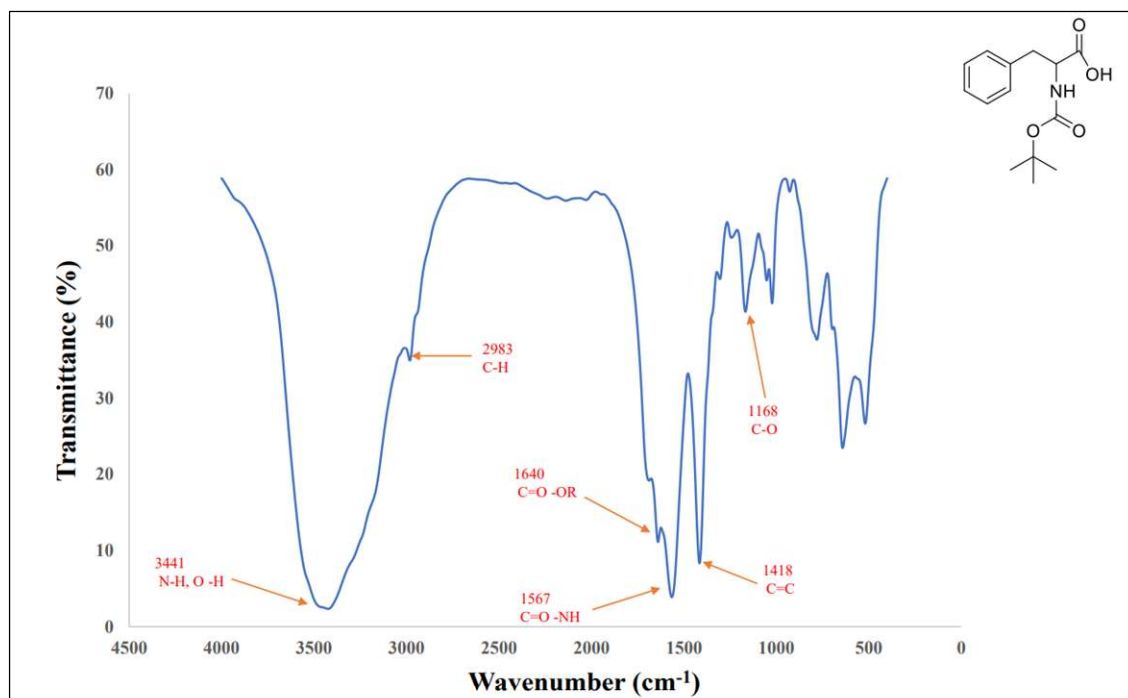


Figure S40. FT-IR spectra of compound (*tert*-butoxycarbonyl)-L-phenylalanine (Boc-*L*-Phe).

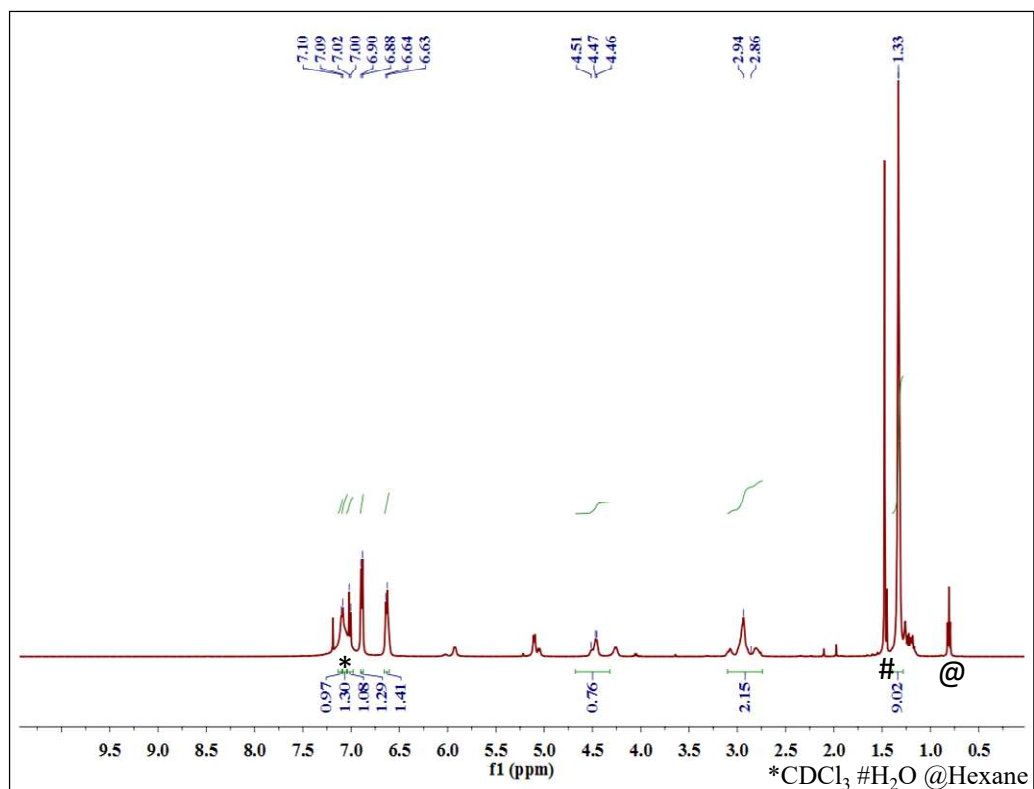


Figure S16. ^1H NMR spectra of compound *(tert-butoxycarbonyl)-L-tyrosine* (Boc-*L*-Tyr).

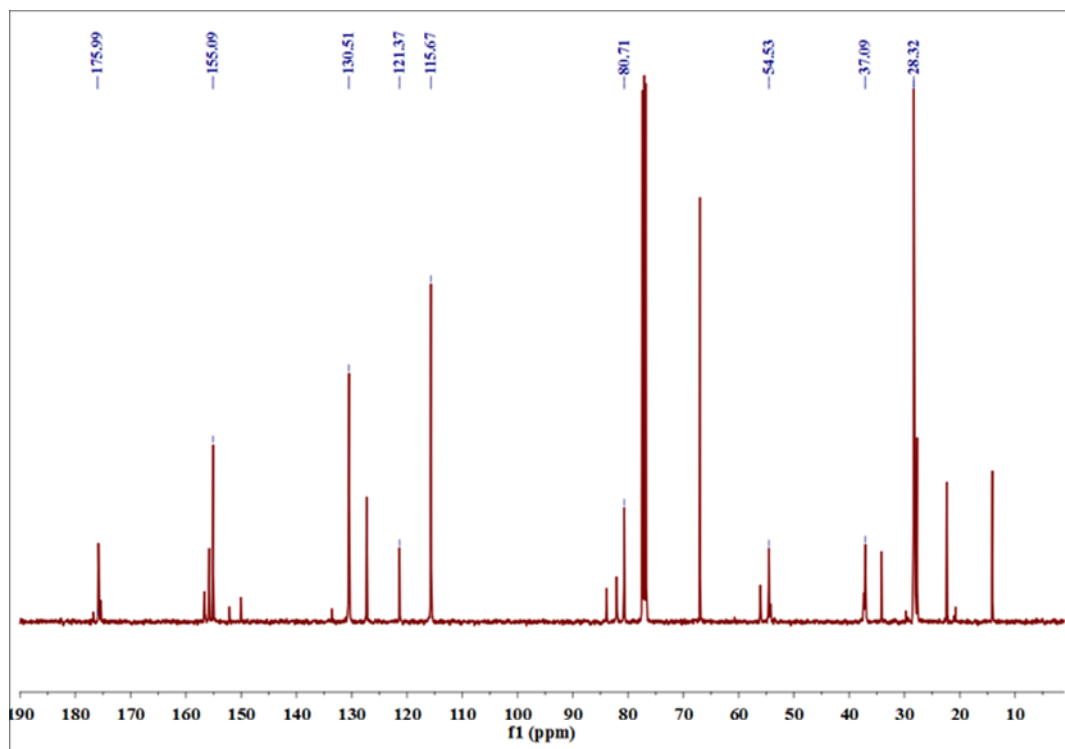


Figure S17. ^{13}C NMR spectra of compound *(tert-butoxycarbonyl)-L-tyrosine* (Boc-*L*-Tyr).

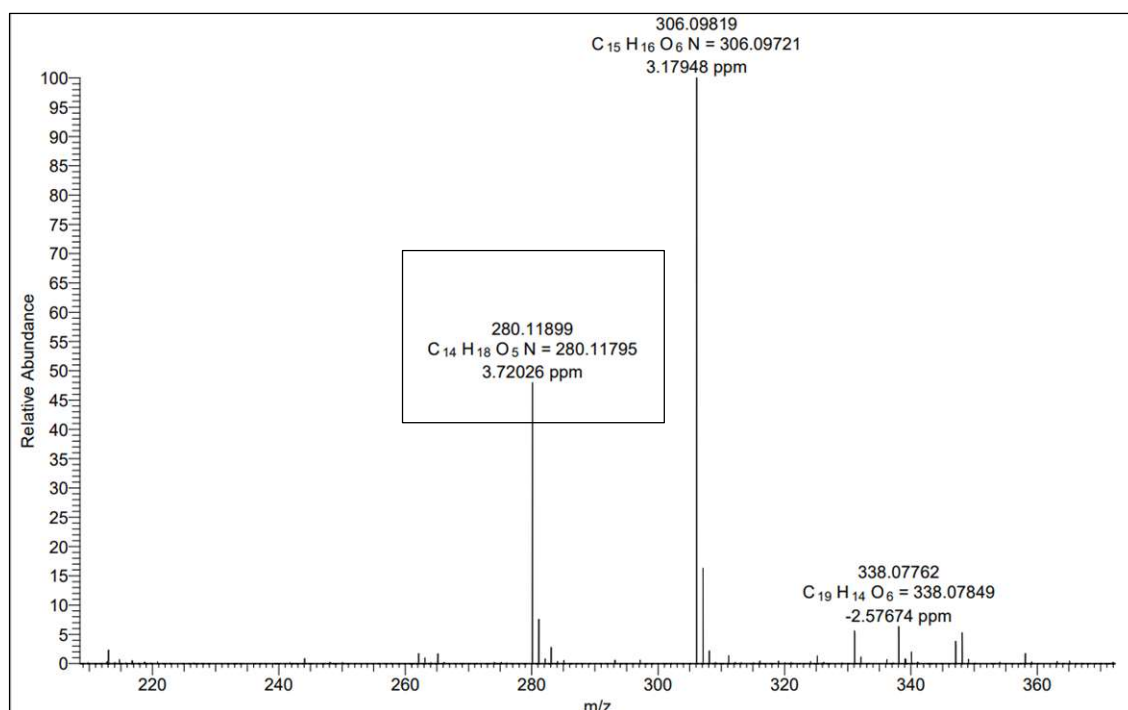


Figure S18. HRMS spectrum of compound (*tert*-butoxycarbonyl)-*L*-tyrosine (Boc-*L*-Tyr).

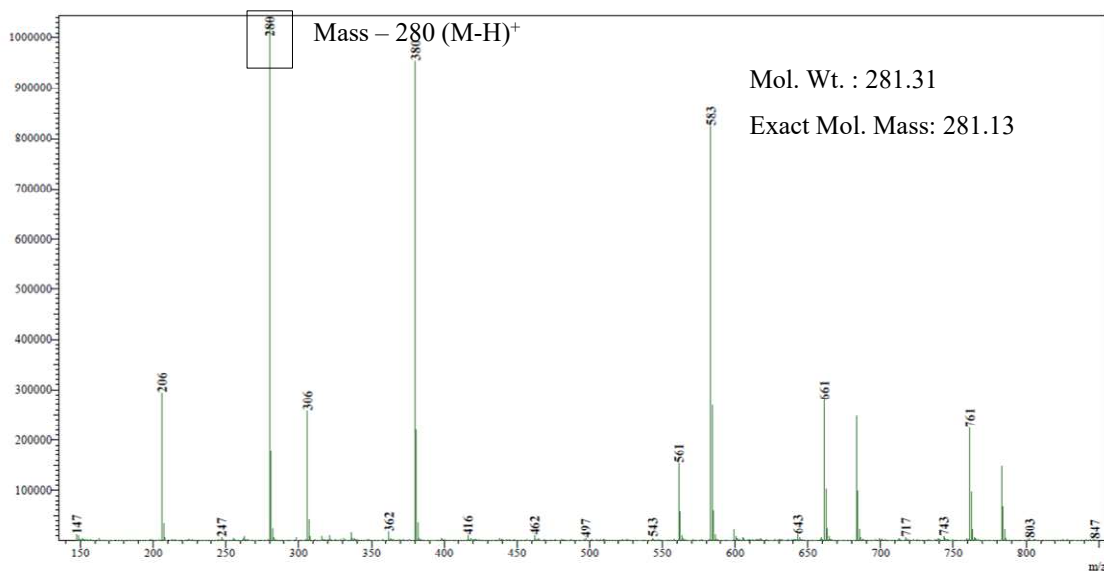


Figure S19. LCMS spectrum of compound (*tert*-butoxycarbonyl)-*L*-tyrosine (Boc-*L*-Tyr).

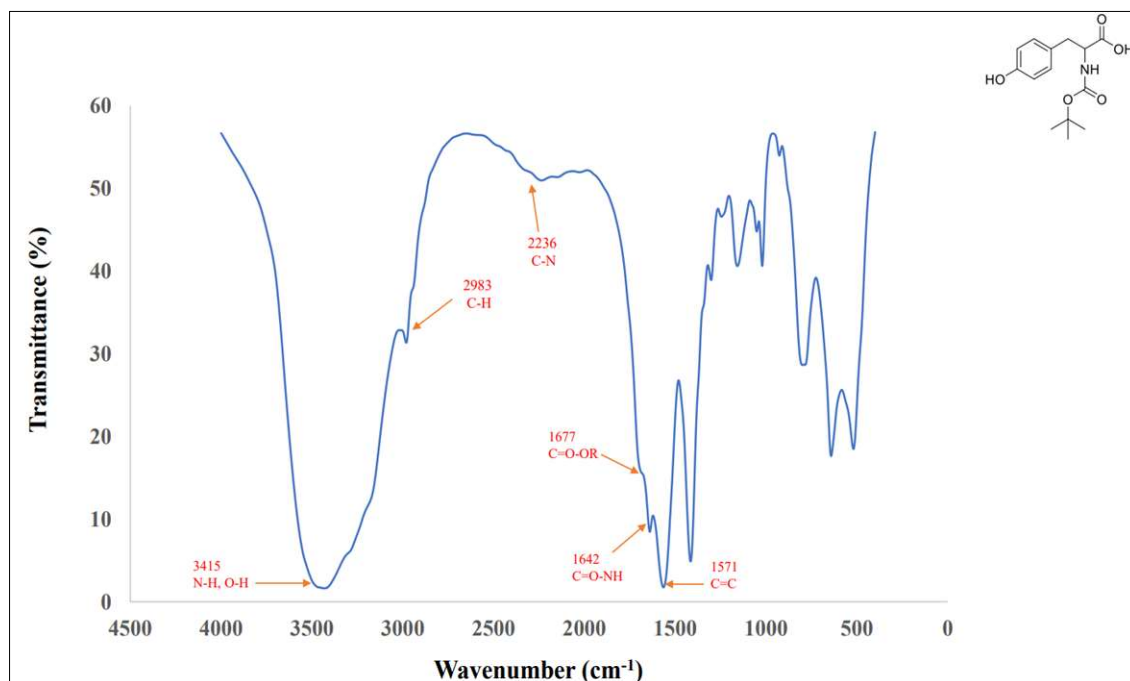


Figure S20. FT-IR spectra of compound (tert-butoxycarbonyl)-L-tyrosine (Boc-L-Tyr).

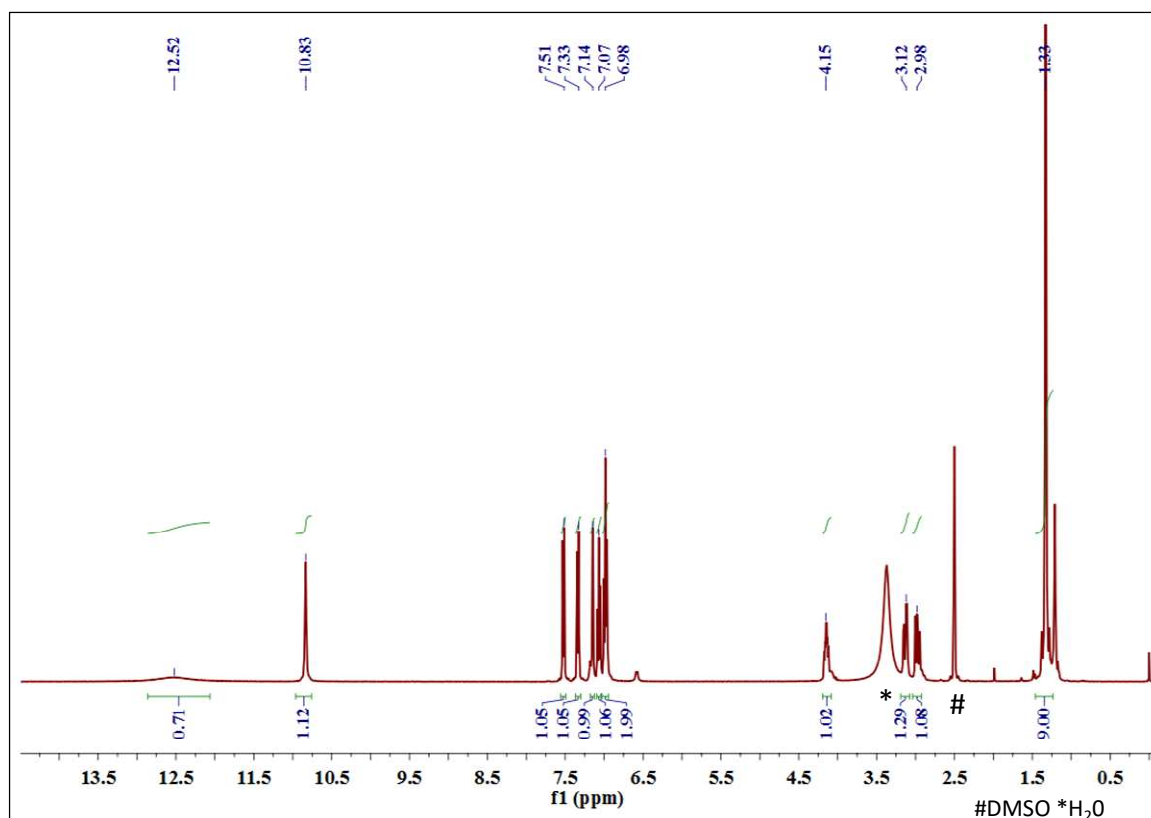


Figure S26. ¹H NMR spectra of compound (tert-butoxycarbonyl)-L-tryptophan (Boc-L-Trp).

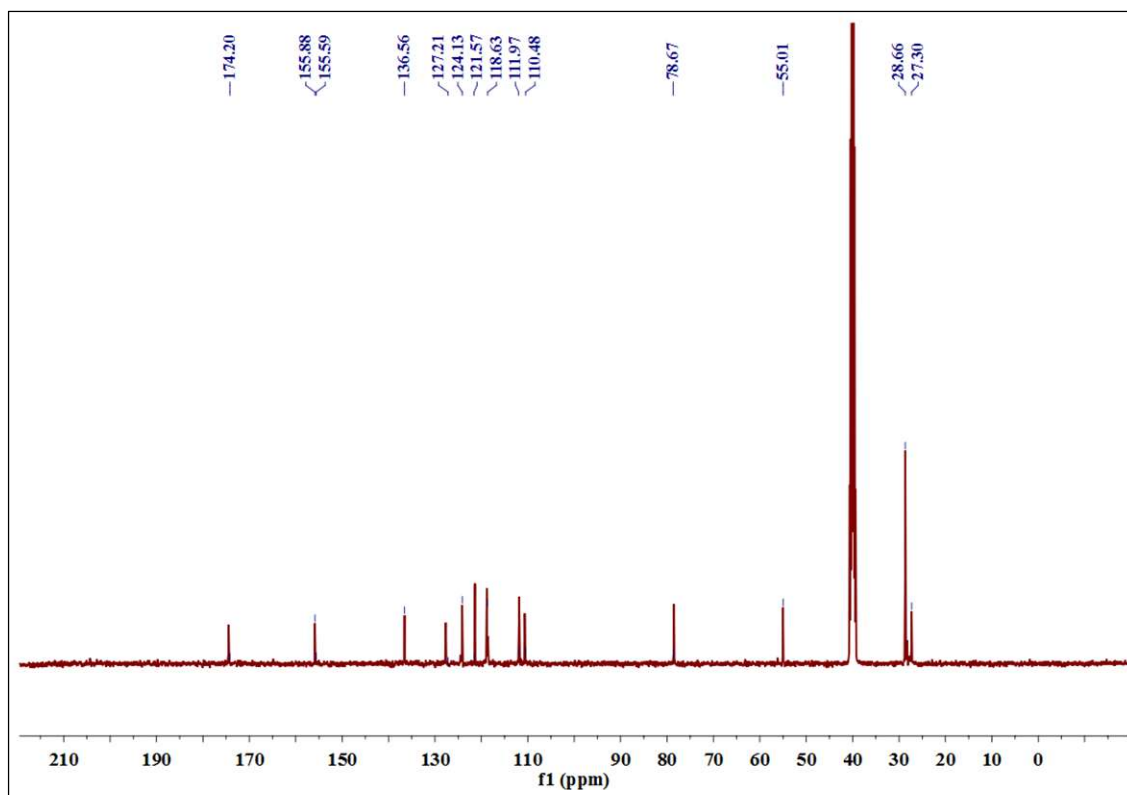


Figure S27. ^{13}C NMR spectra of compound (*tert*-butoxycarbonyl)-*L*-tryptophan (Boc-*L*-Trp).

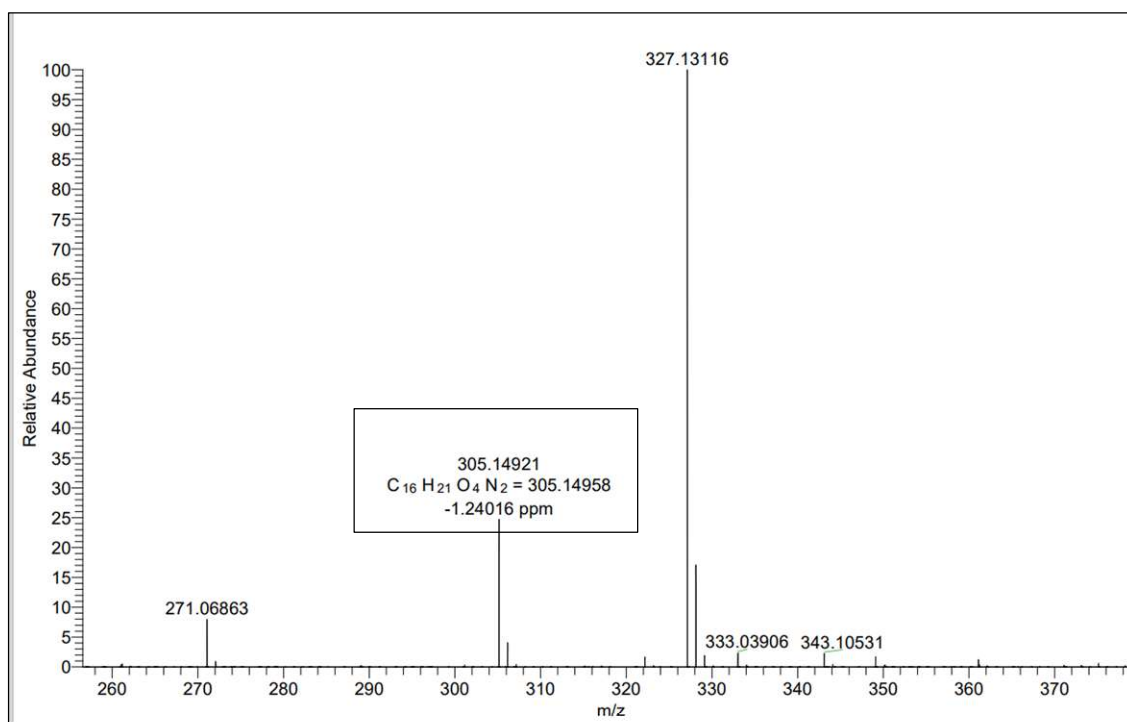


Figure S28. HRMS spectrum of compound (*tert*-butoxycarbonyl)-*L*-tryptophan (Boc-*L*-Trp).

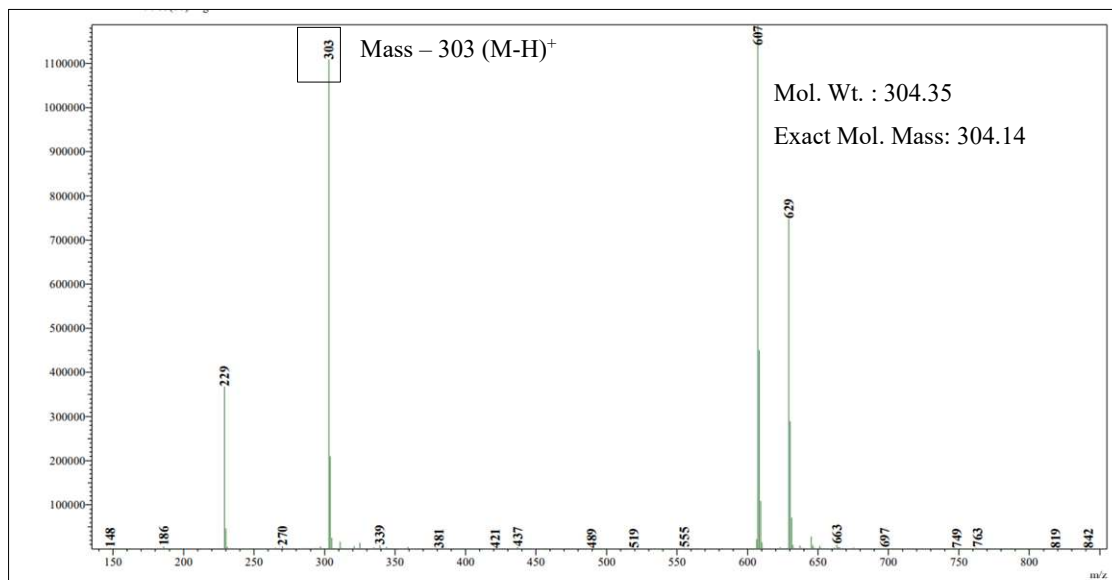


Figure S29. LCMS spectrum of compound (*tert*-butoxycarbonyl)-*L*-tryptophan (Boc-*L*-Trp).

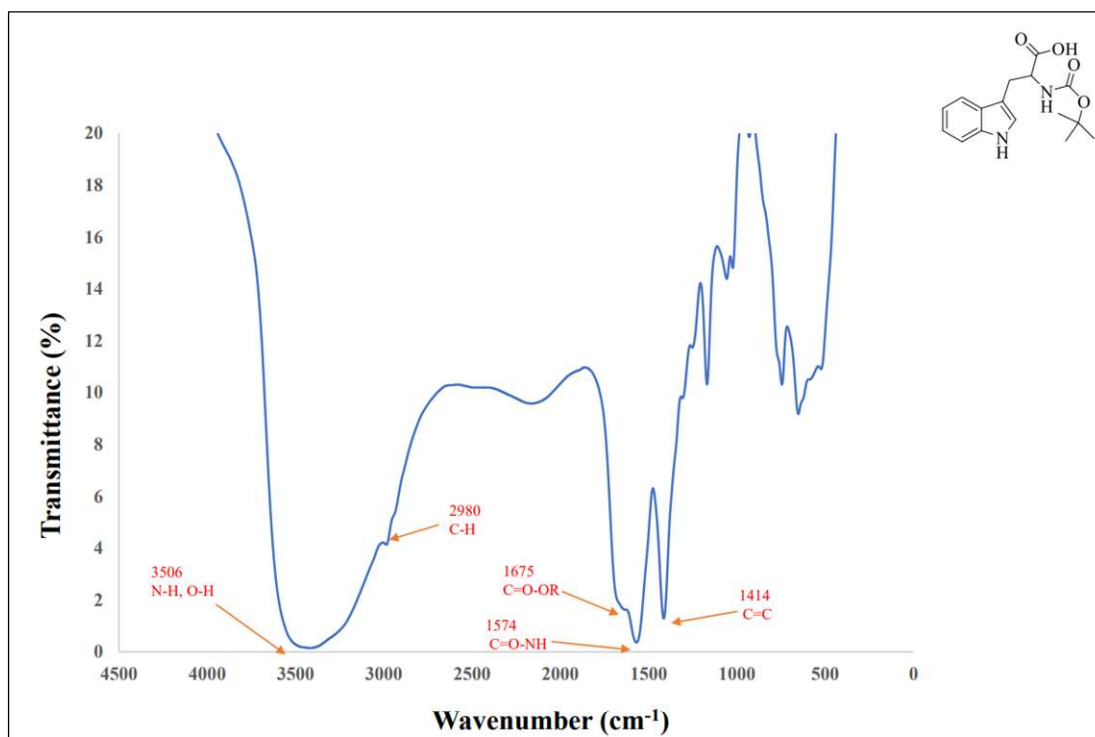


Figure S30. FT-IR spectra of compound (*tert*-butoxycarbonyl)-*L*-tryptophan (Boc-*L*-Trp).

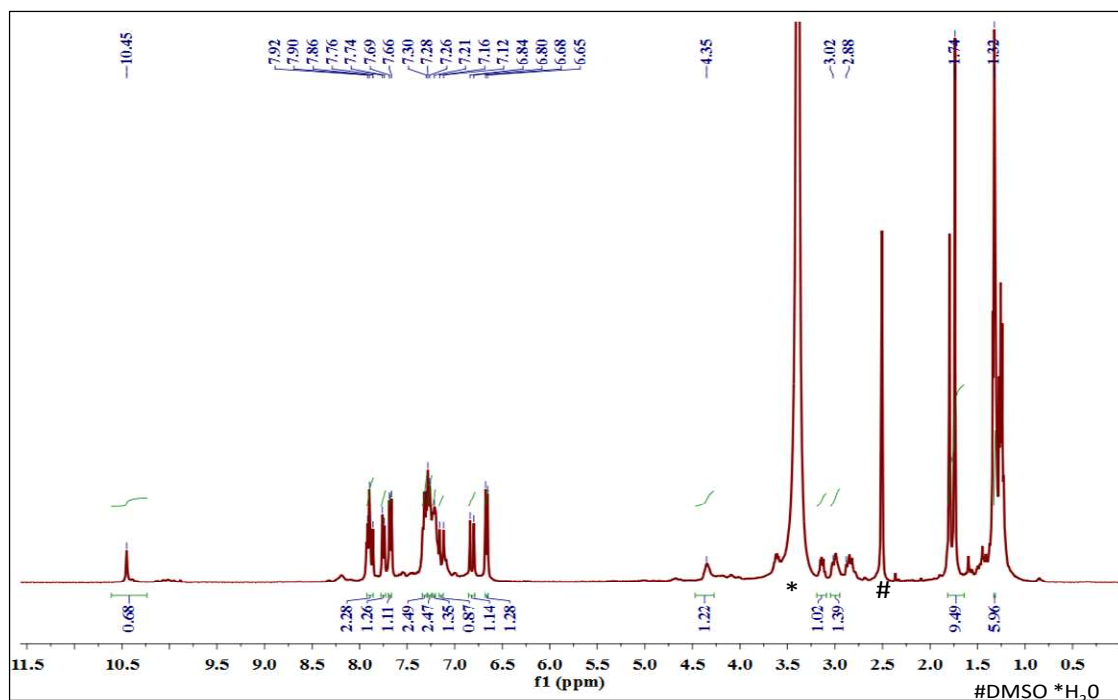


Figure S41. ¹H NMR spectra of compound Boc-*L*-Phe-TCF-1.

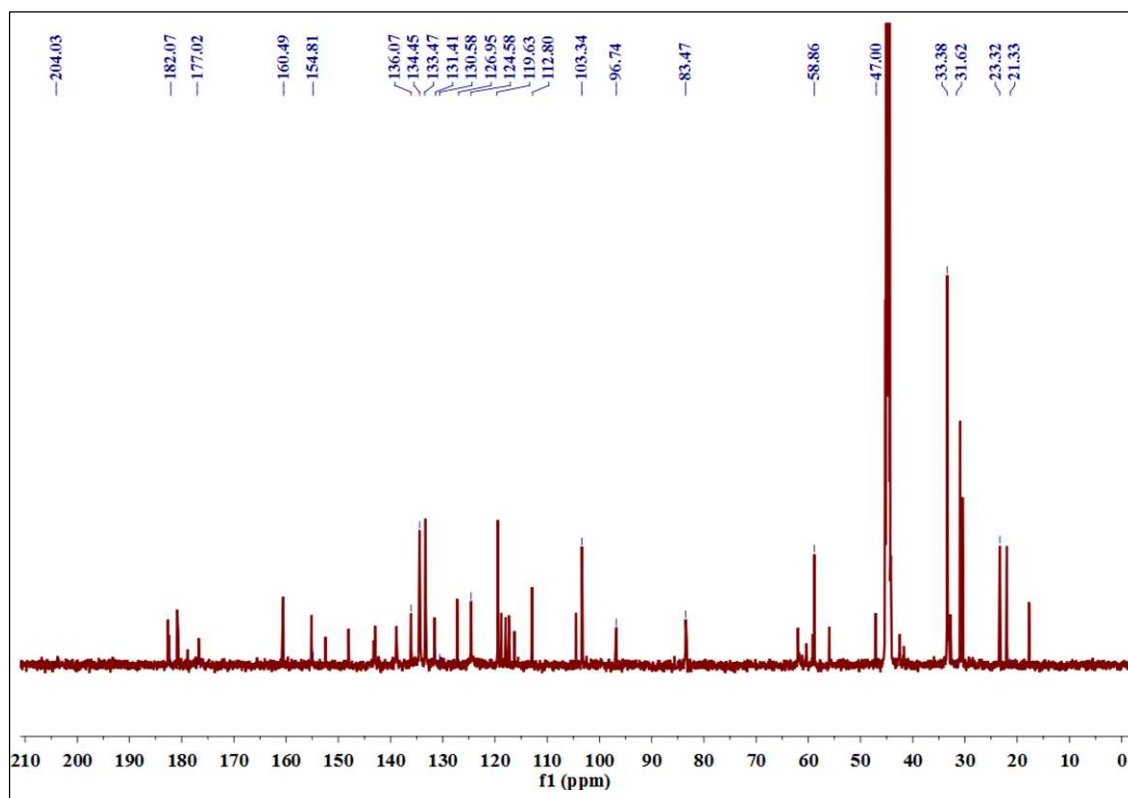


Figure S42. ¹³C NMR spectra of compound Boc-*L*-Phe-TCF-1.

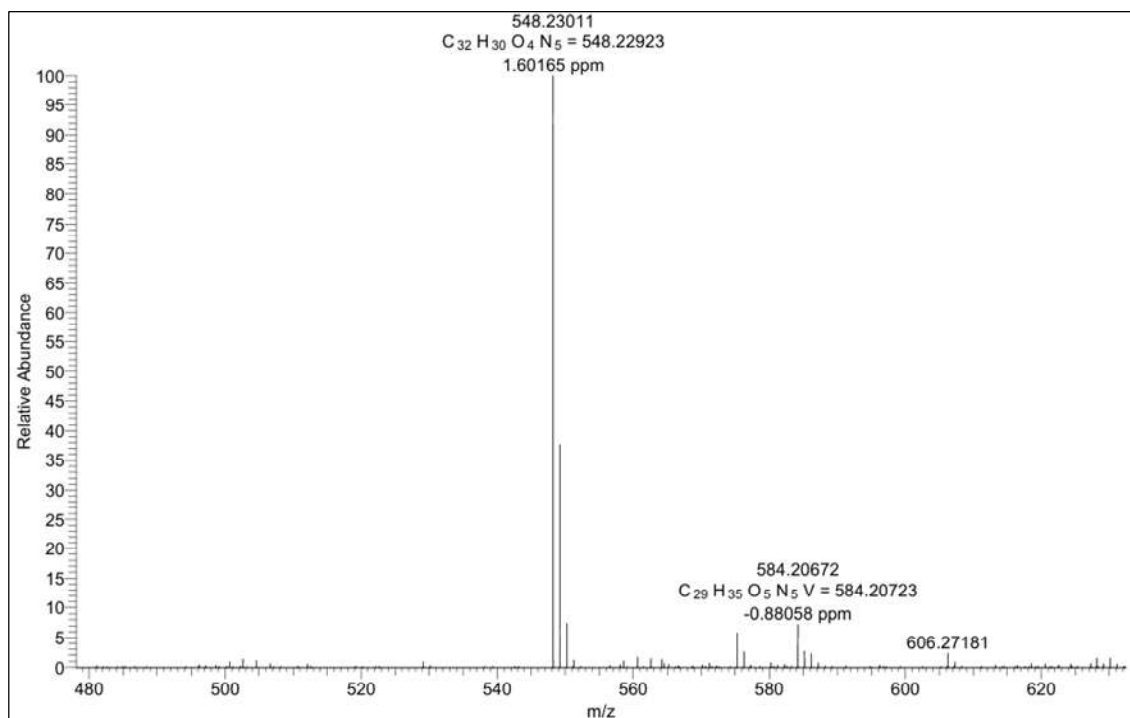


Figure S43. HRMS spectrum of compound Boc-*L*-Phe-TCF-1.

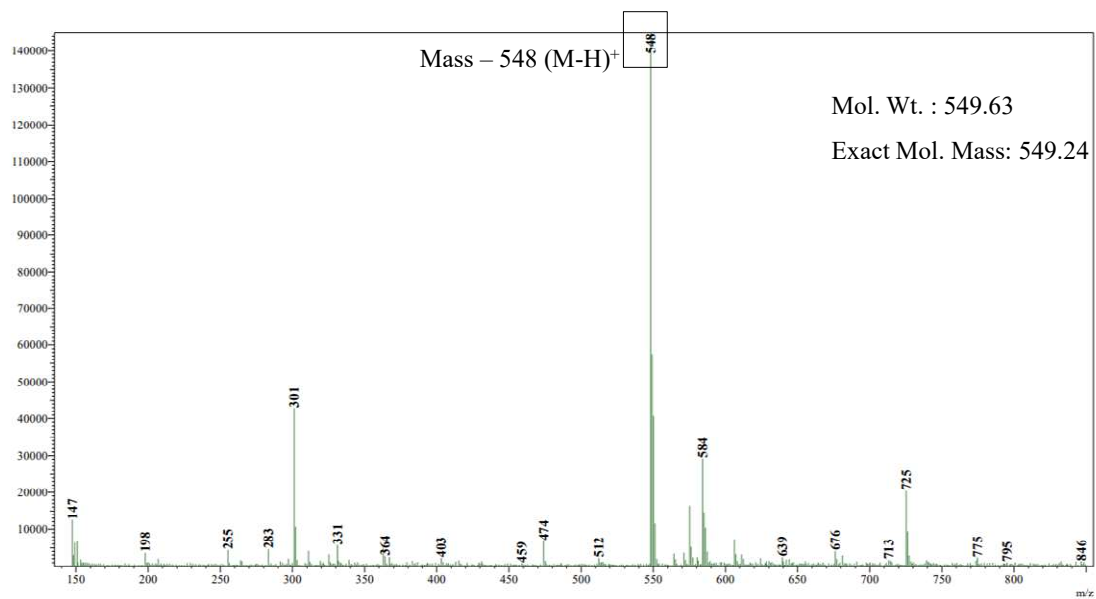


Figure S44. LCMS spectrum of compound Boc-*L*-Phe-TCF-1.

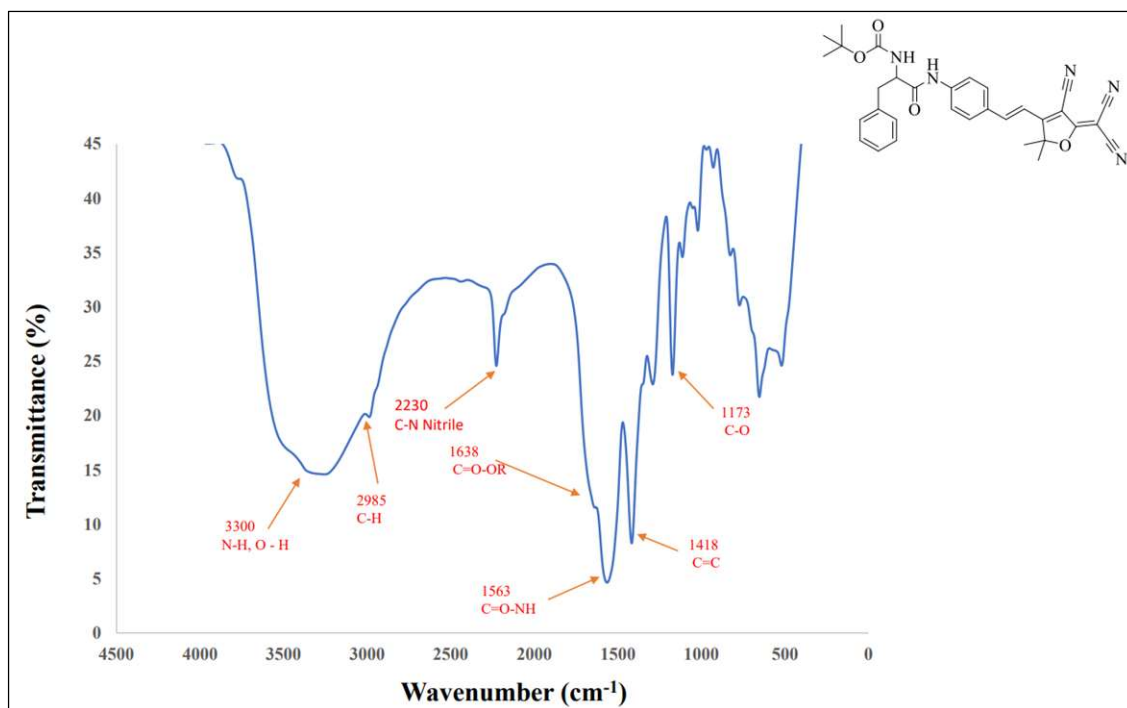


Figure S45. FT-IR spectra of compound Boc-L-Phe-TCF-1.

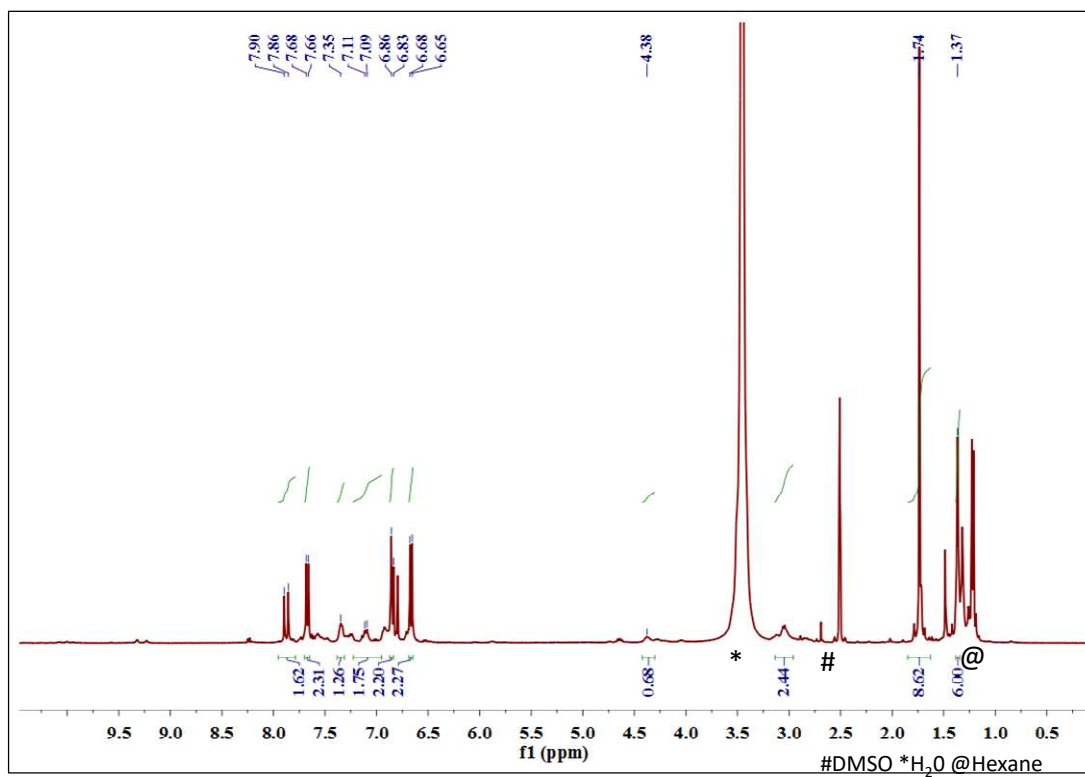


Figure S21. ¹H NMR spectra of compound Boc-L-Tyr-TCF-1.

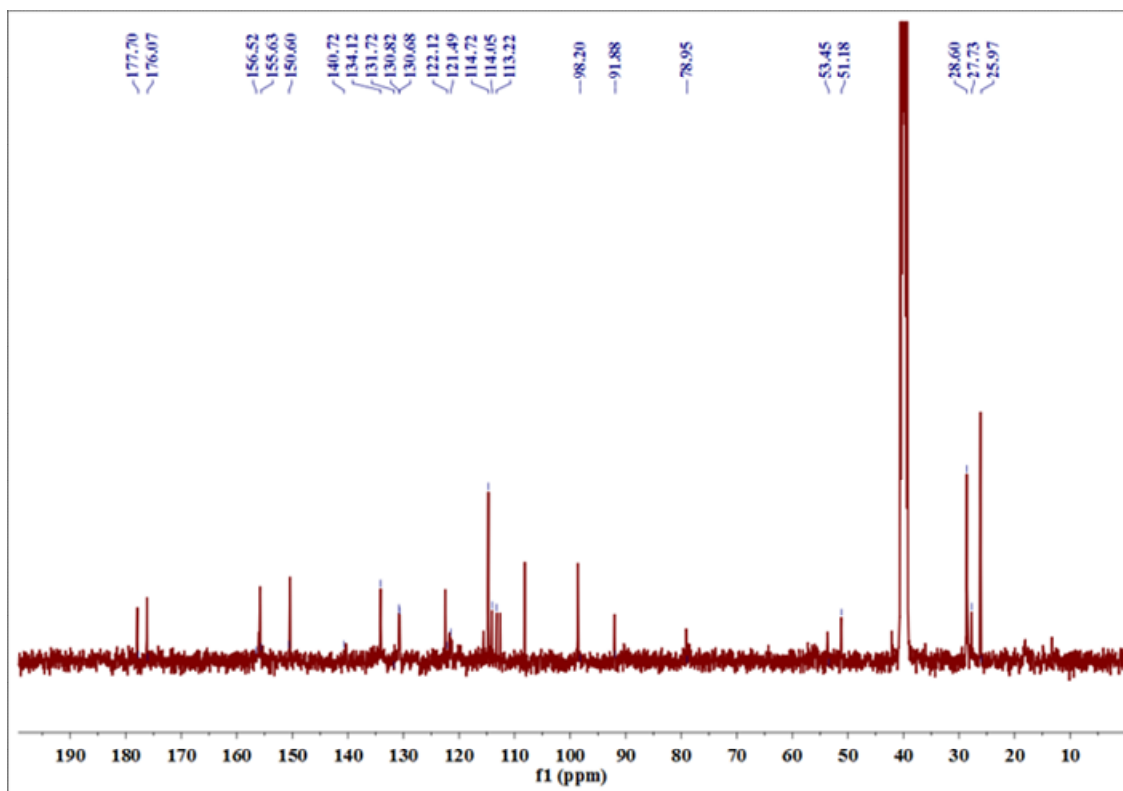


Figure S22. ^{13}C NMR spectra of compound Boc-*L*-Tyr-TCF-1.

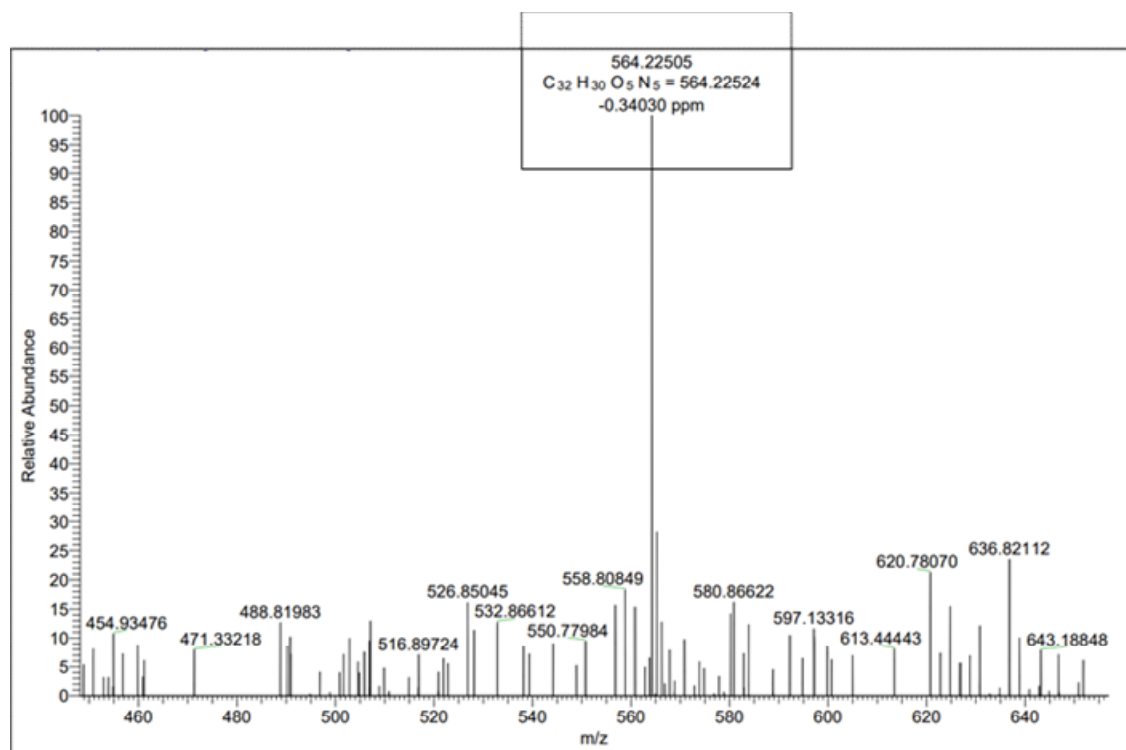


Figure S23. HRMS spectrum of compound Boc-*L*-Tyr-TCF-1.

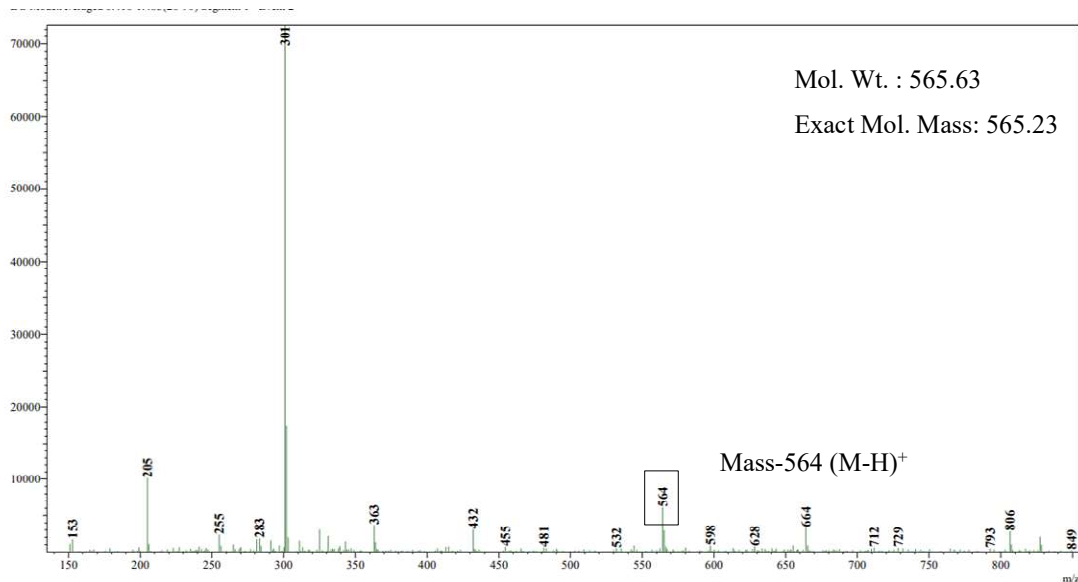


Figure S24. LCMS spectrum of compound Boc-*L*-Tyr-TCF-1.

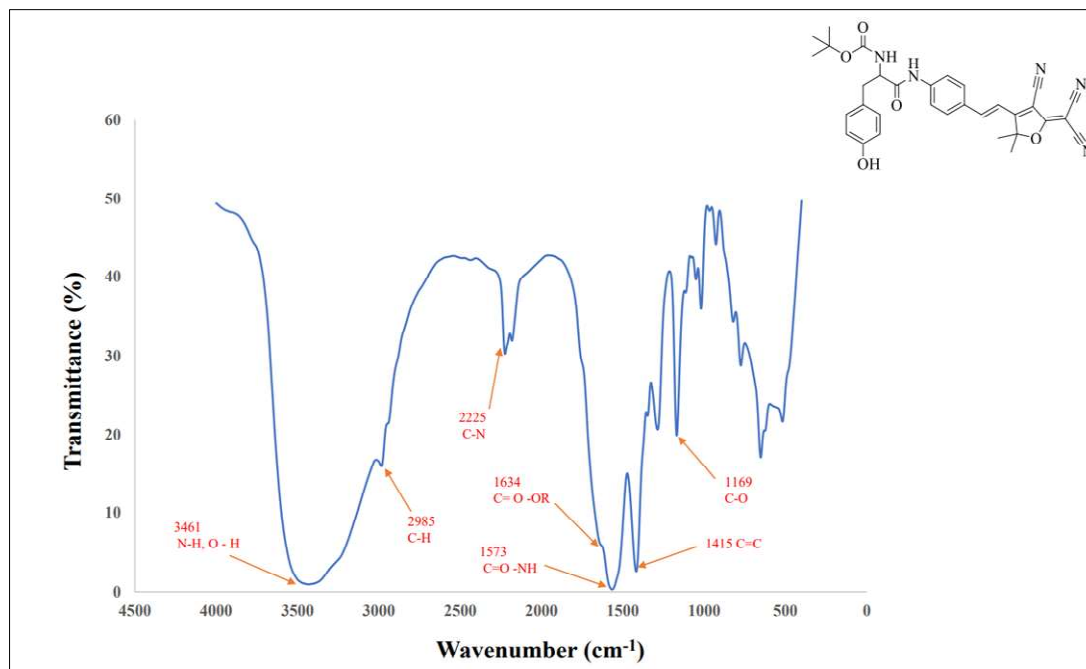


Figure S25. FT-IR spectra of compound Boc-*L*-Tyr-TCF-1.

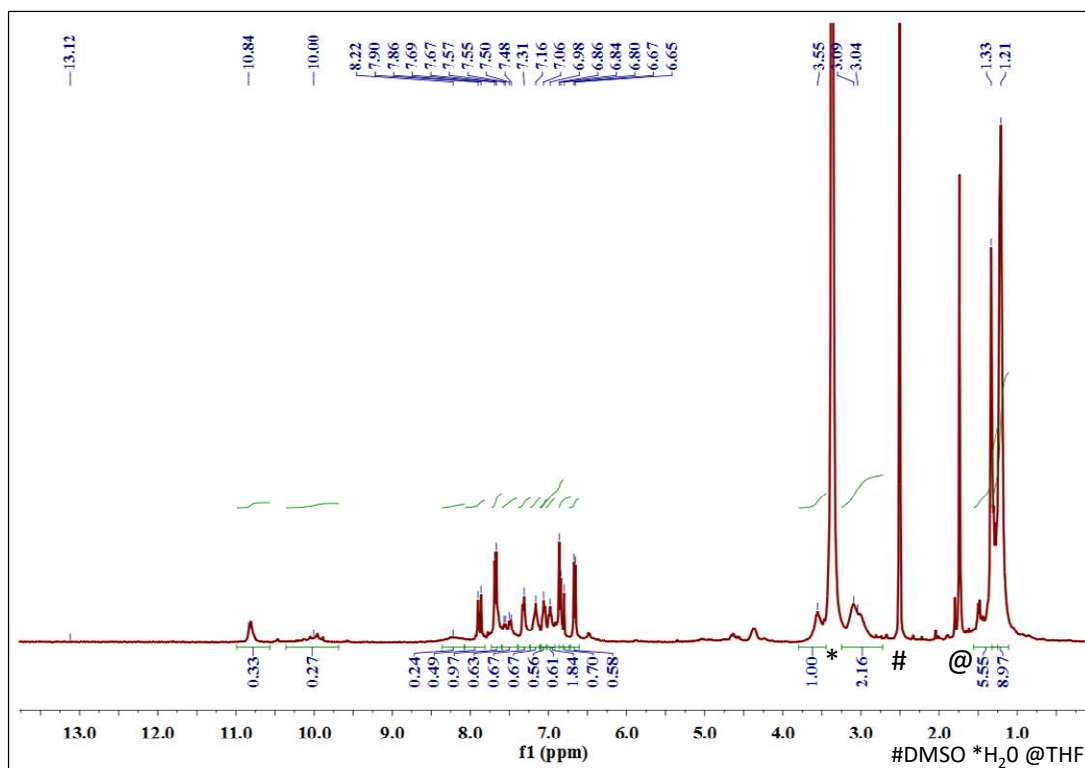


Figure S31. ^1H NMR spectra of compound Boc-*L*-Trp-TCF-1.

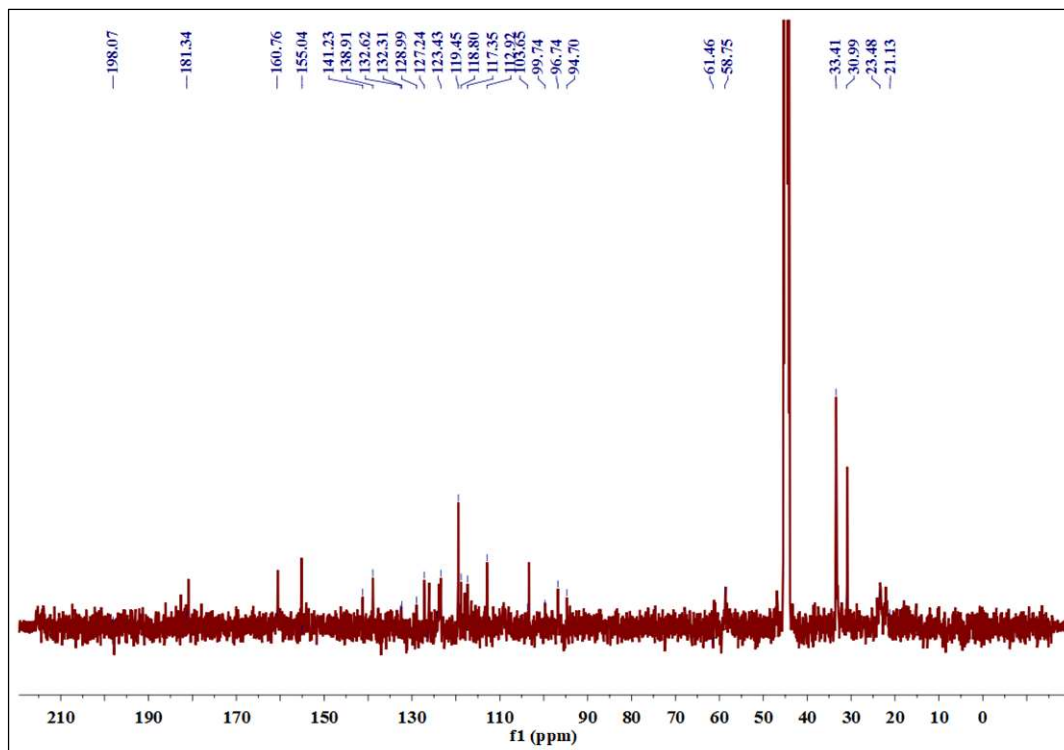


Figure S32. ^{13}C NMR spectra of compound Boc-*L*-Trp-TCF-1.

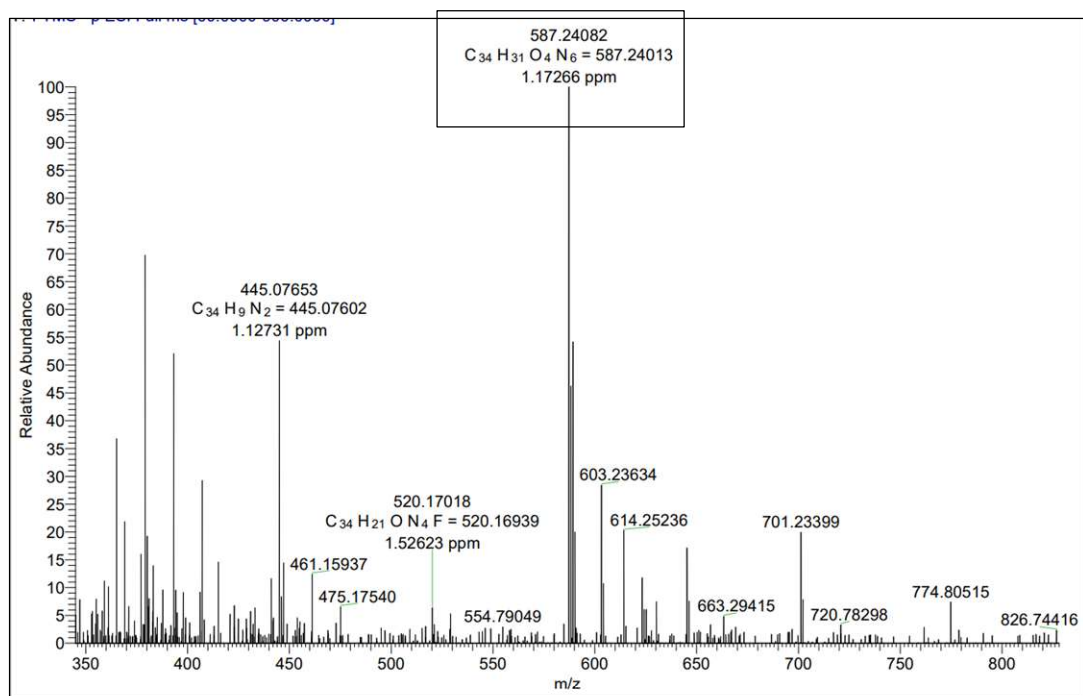


Figure S33. HRMS spectrum of compound Boc-L-Trp-TCF-1.

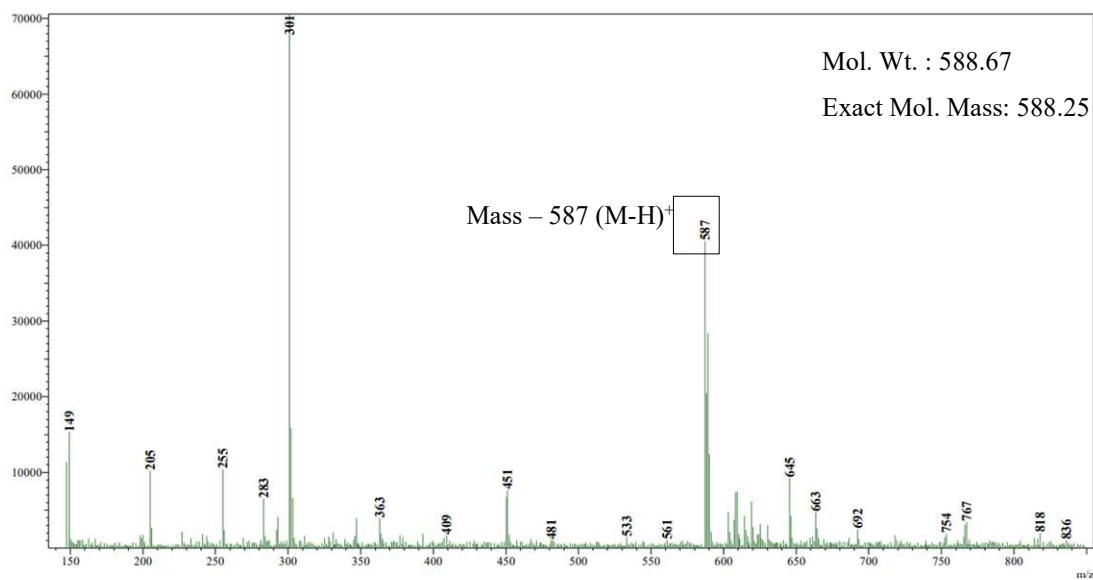


Figure S34. LCMS spectrum of compound Boc-L-Trp-TCF-1.

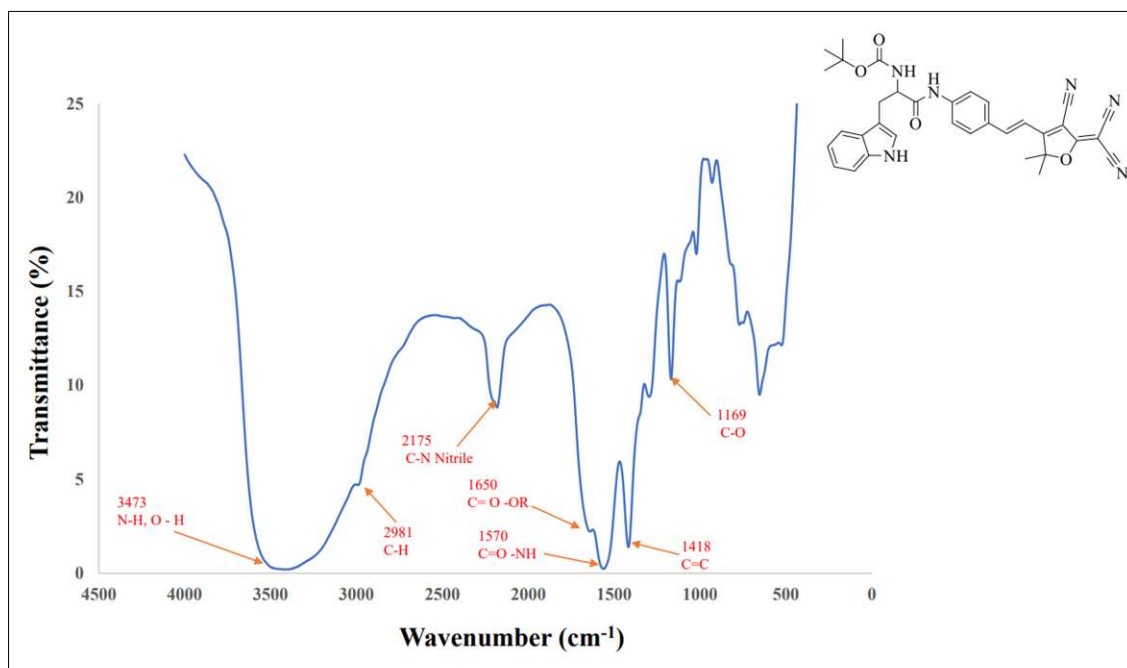


Figure S35. FT-IR spectra of compound Boc-L-Trp-TCF-1.

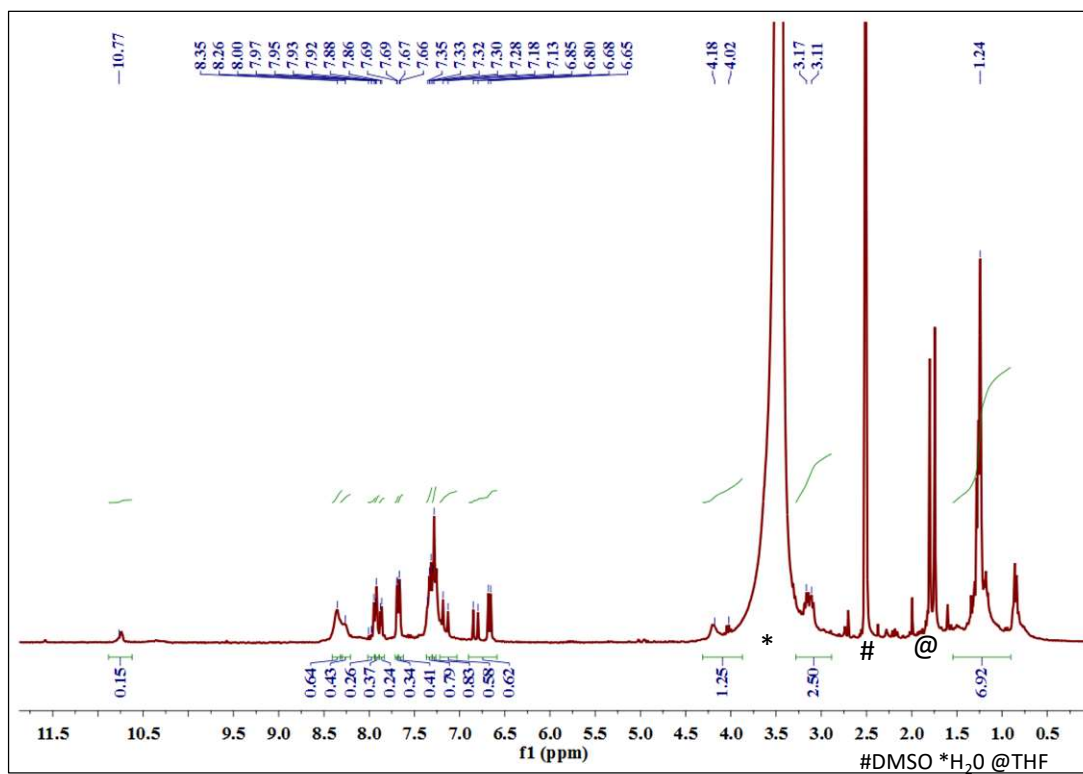


Figure S56. ¹H NMR spectra of compound L-Phe-TCF-1.

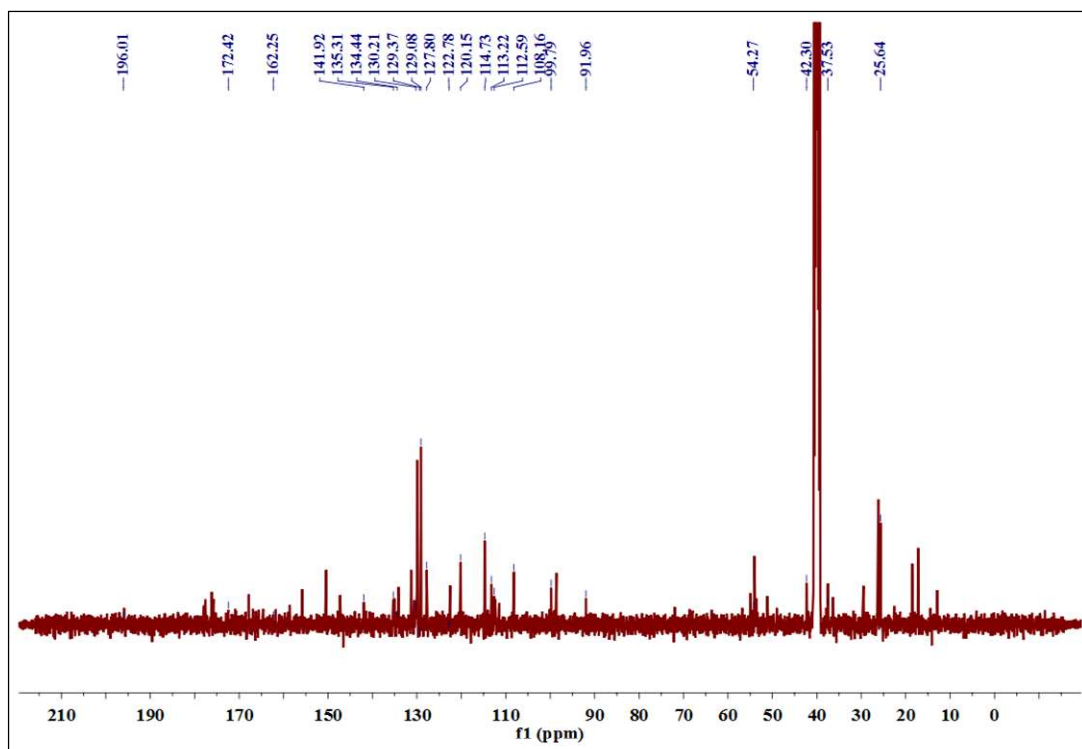


Figure S57. ^{13}C NMR spectra of compound *L*-Phe-TCF-1.

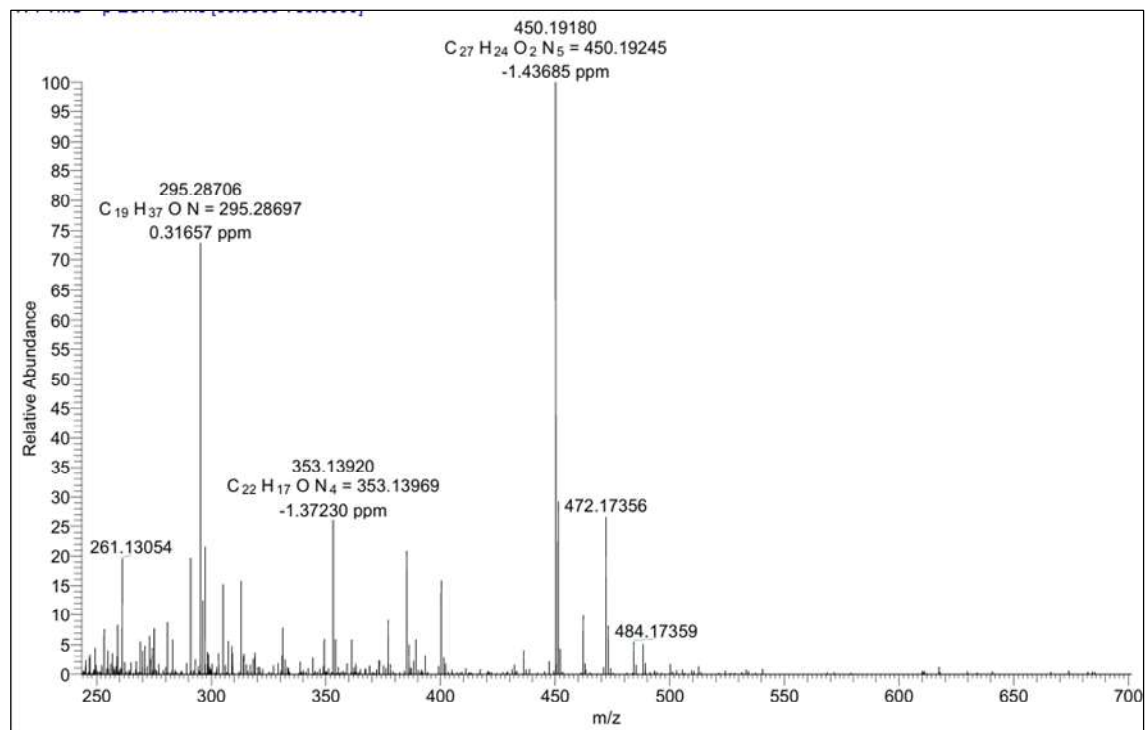


Figure S58. HRMS spectrum of compound *L*-Phe-TCF-1.

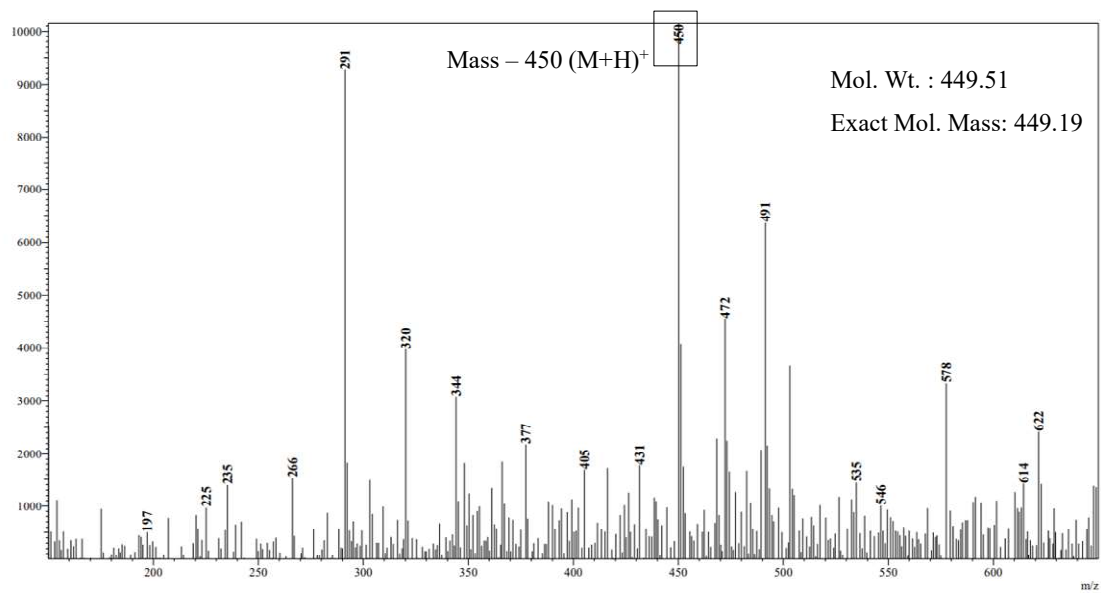


Figure S59. LCMS spectrum of compound *L*-Phe-TCF-1.

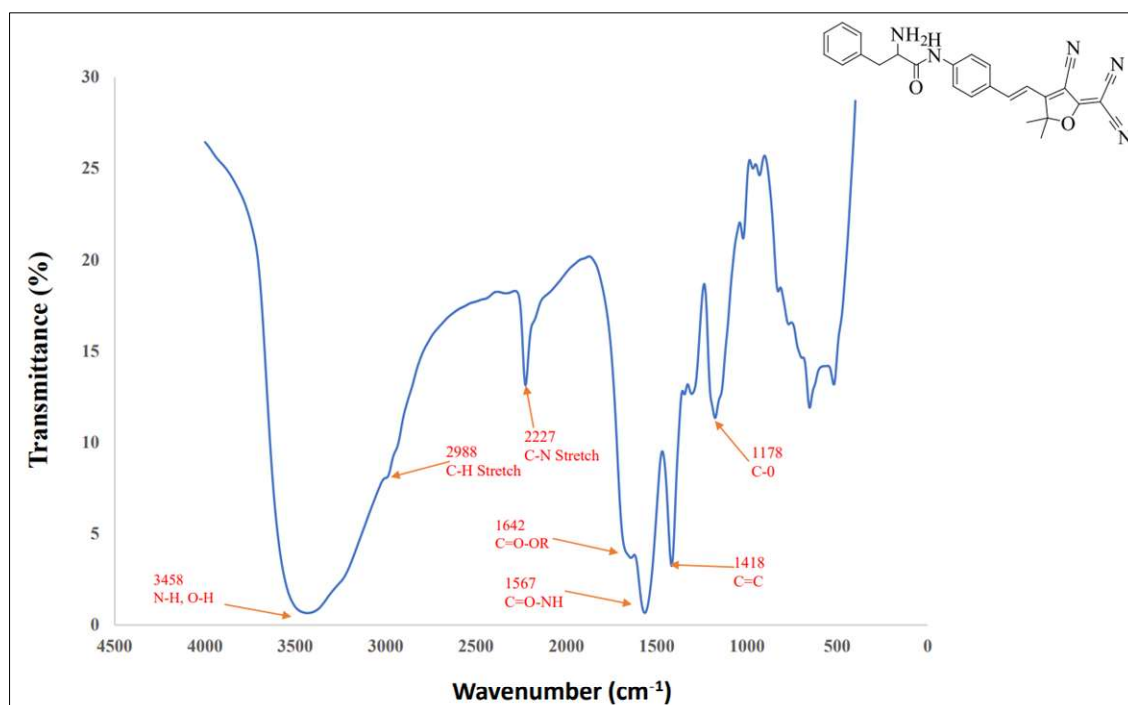


Figure S60. FT-IR spectra of compound *L*-Phe-TCF-1.

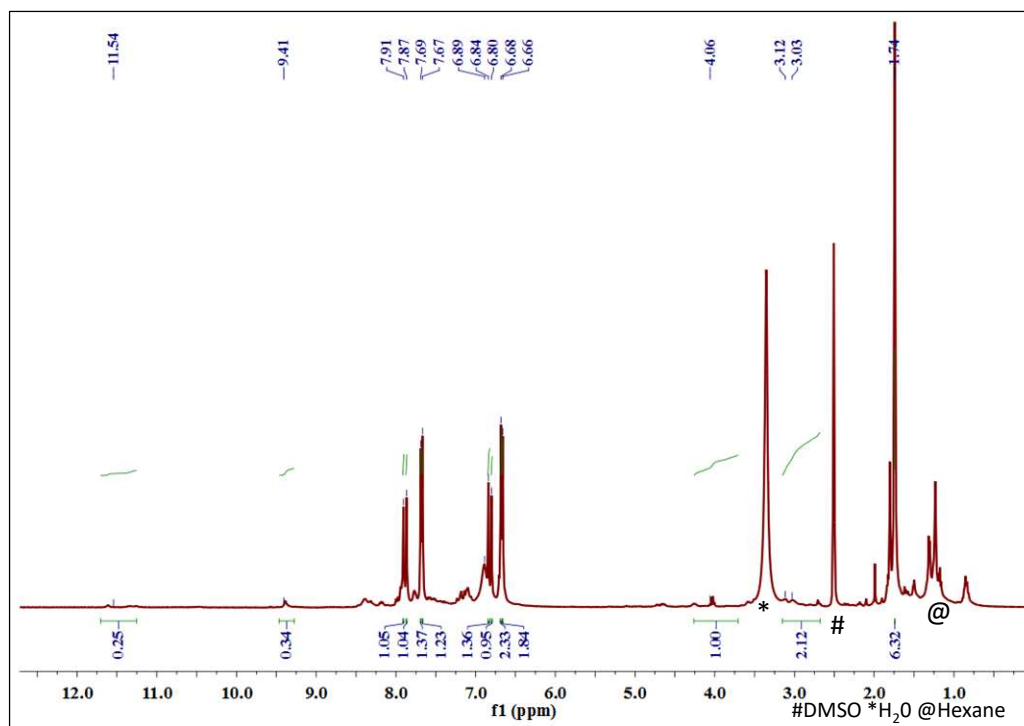


Figure S46. ¹H NMR spectra of compound *L*-Tyr-TCF-1.

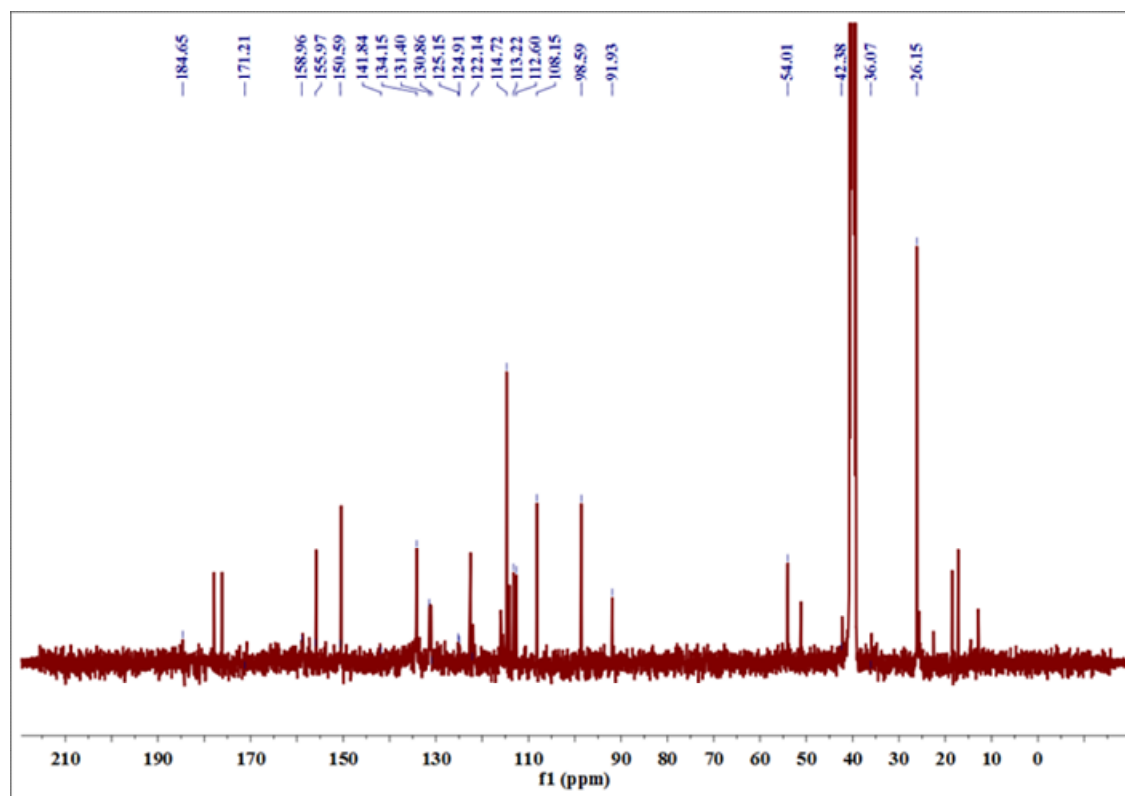


Figure S47. ¹³C NMR spectra of compound *L*-Tyr-TCF-1.

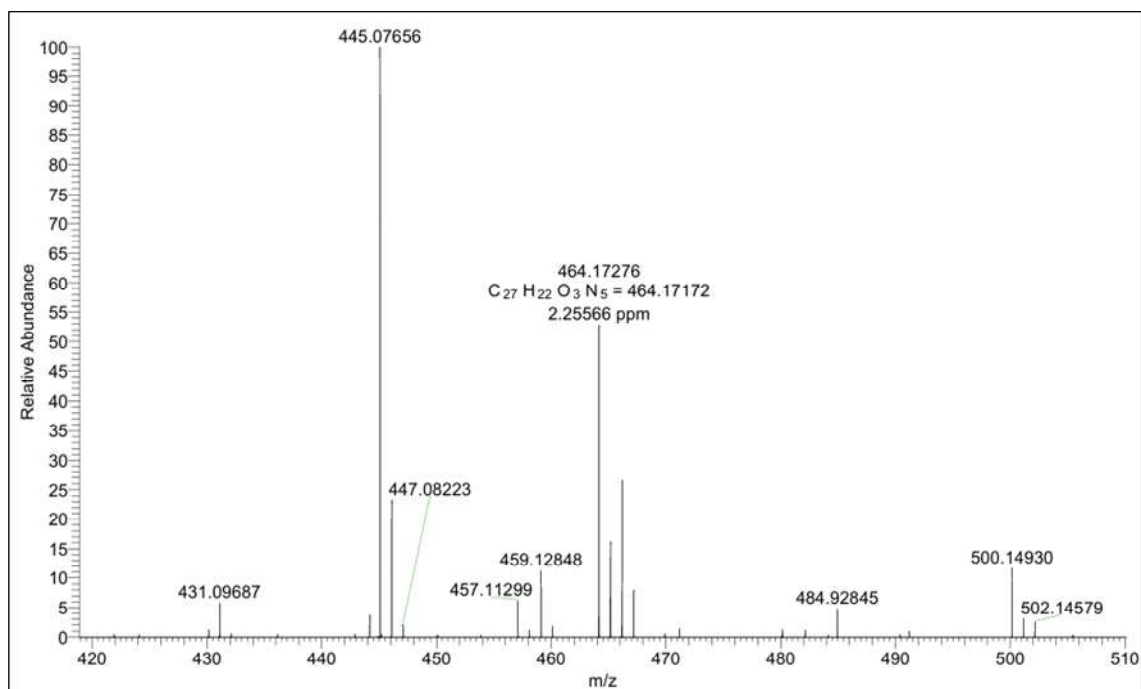


Figure S48. HRMS spectrum of compound *L*-Tyr-TCF-1.

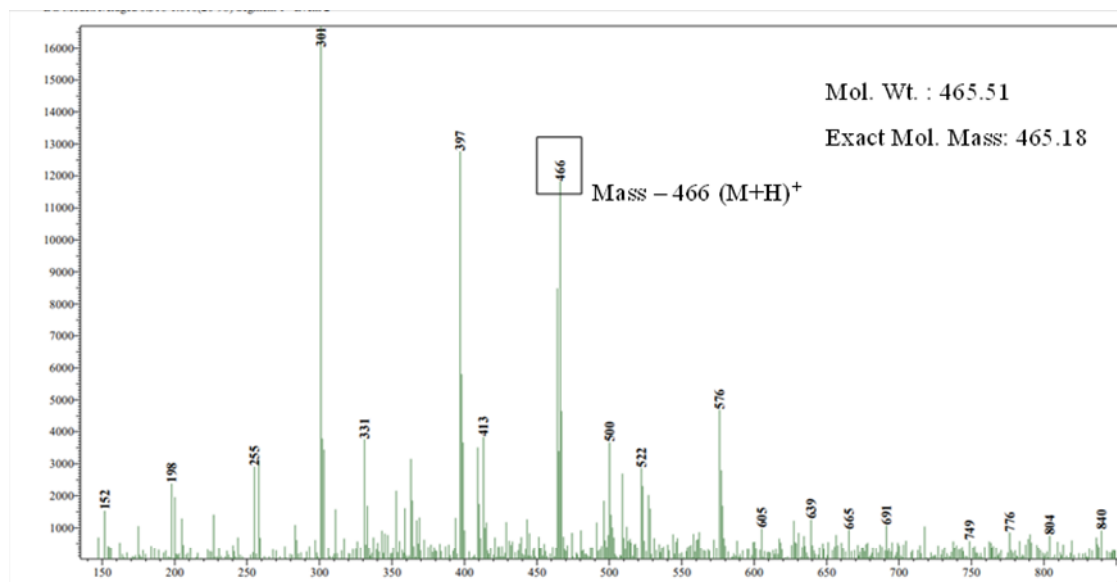


Figure S49. LCMS spectrum of compound *L*-Tyr-TCF-1.

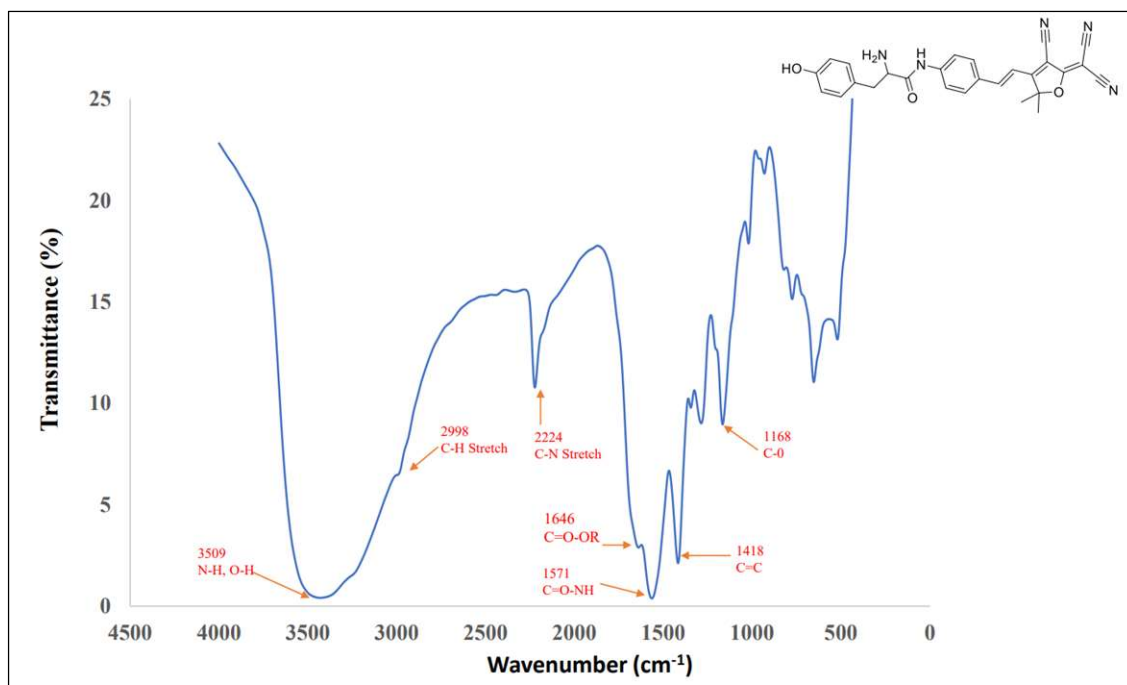


Figure S50. FT-IR spectra of compound *L*-Tyr-TCF-1.

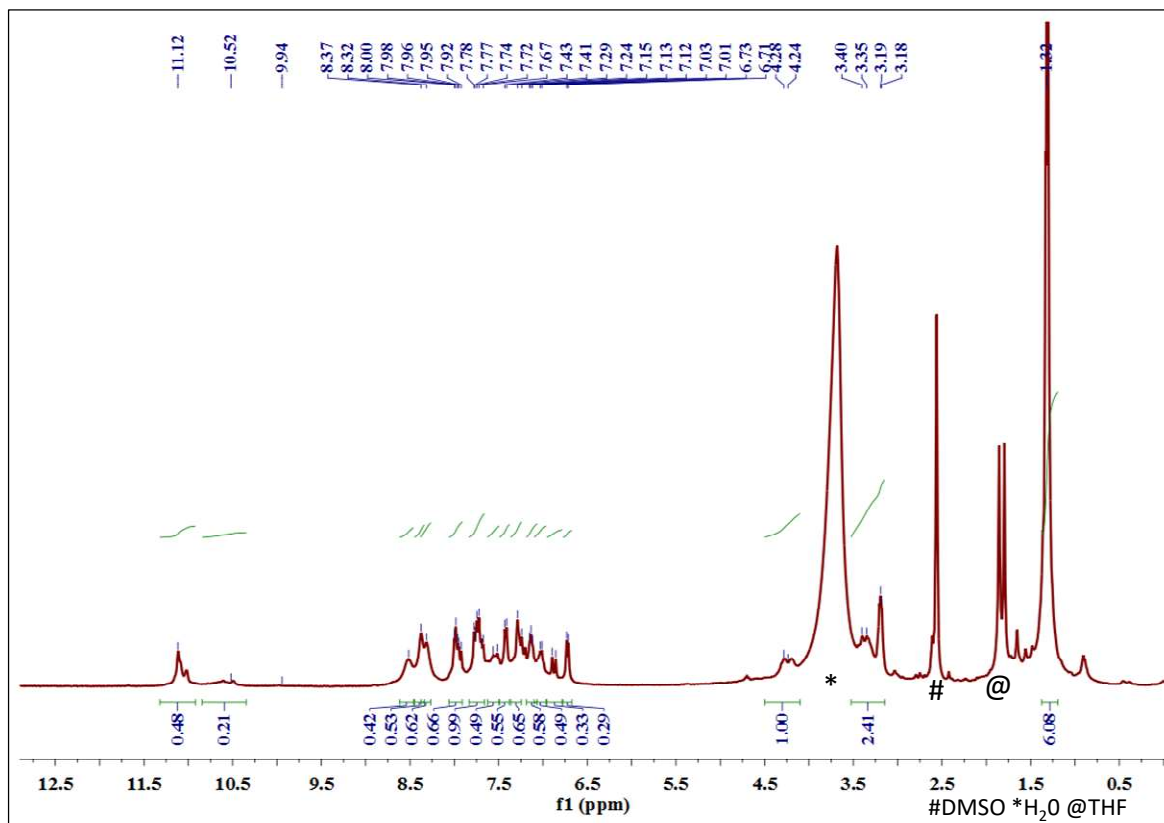


Figure S51. ¹H NMR spectra of compound *L*-Trp-TCF-1.

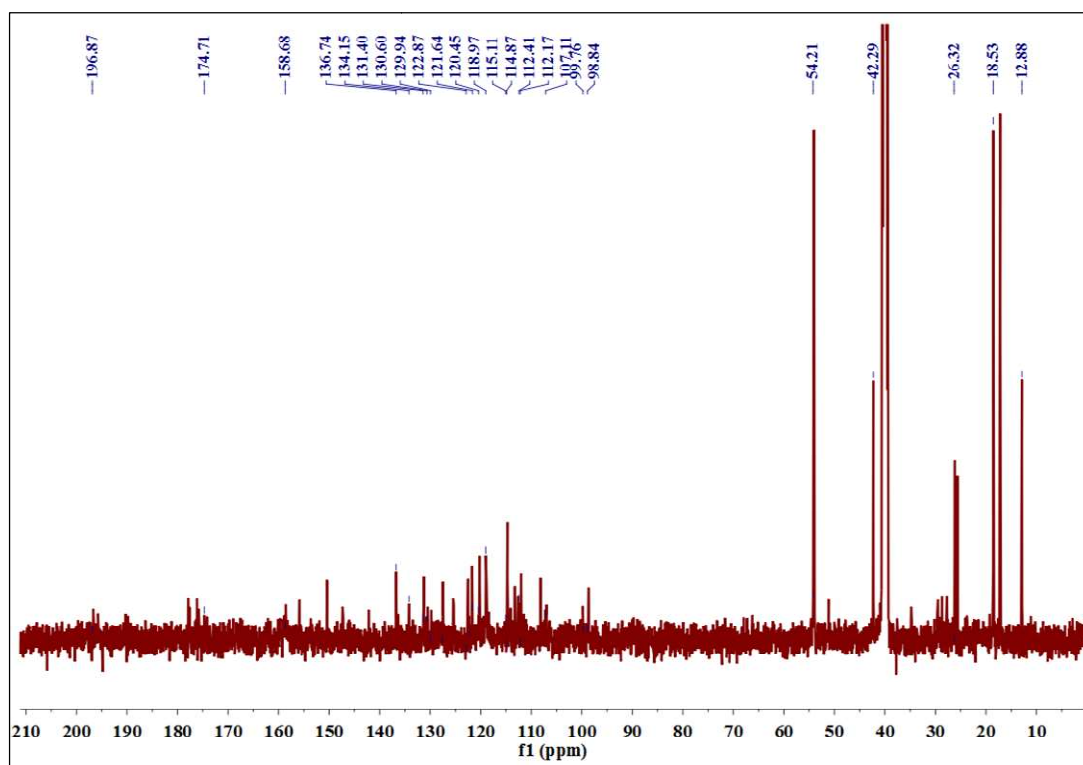


Figure S52. ^{13}C NMR spectra of compound *L*-Trp-TCF-1.

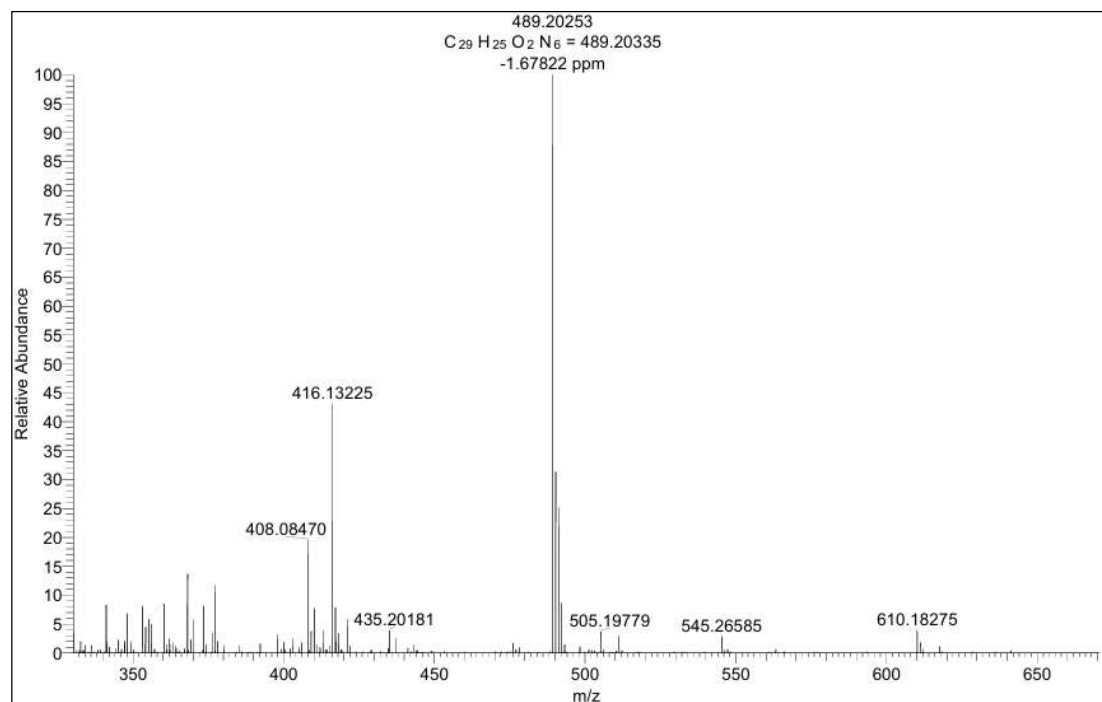


Figure S53. HRMS spectrum of compound *L*-Trp-TCF-1.

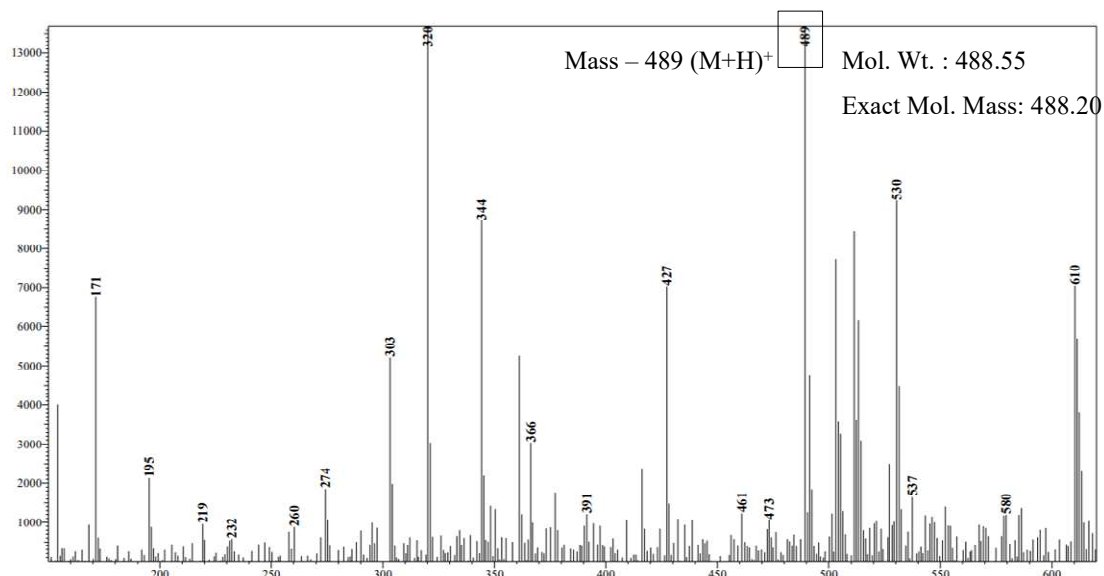


Figure S54. LCMS spectrum of compound *L*-Trp-TCF-1.

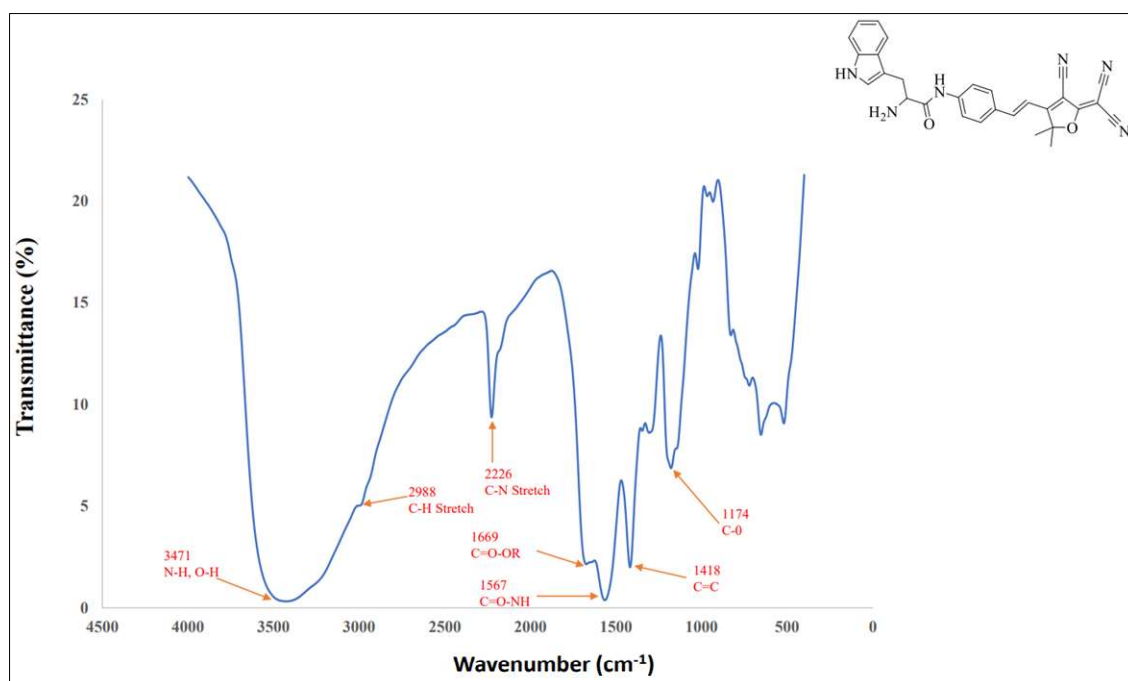


Figure S55. FT-IR spectra of compound *L*-Trp-TCF-1.

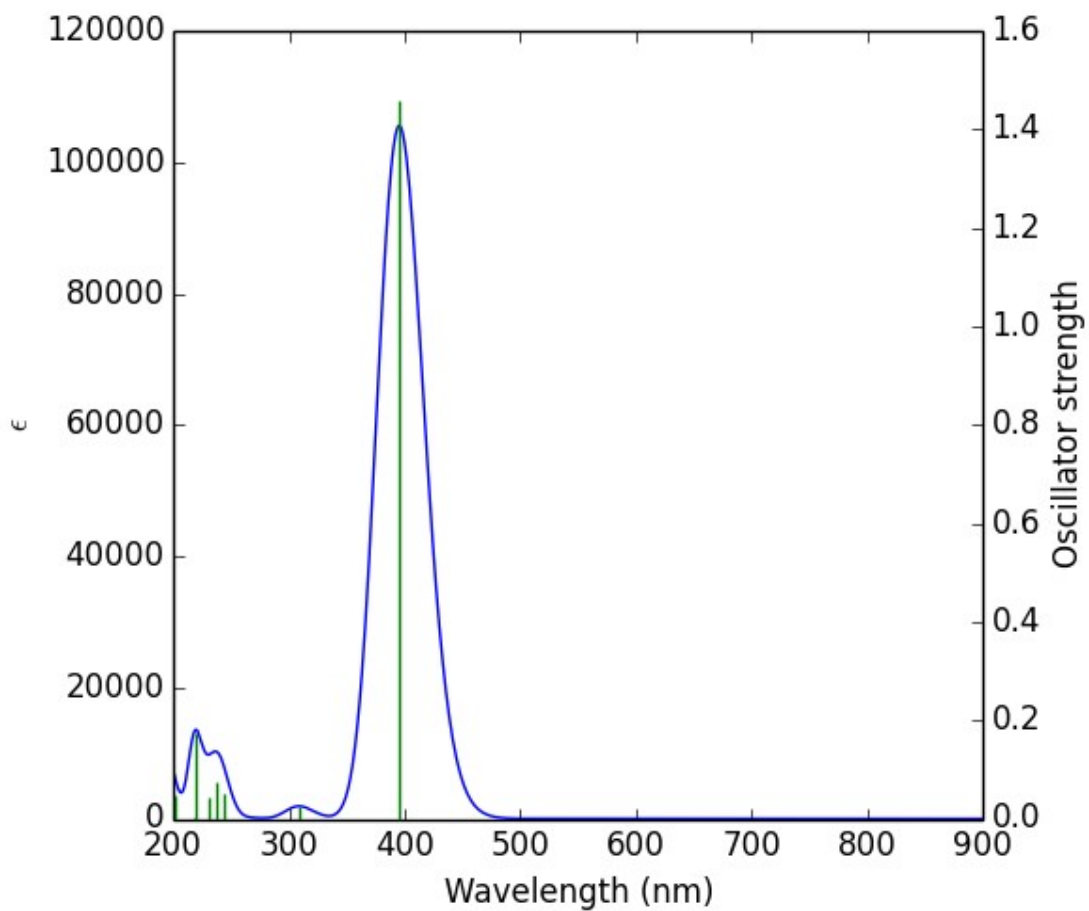


Figure S56. The computed absorption spectrum of TCF-1.

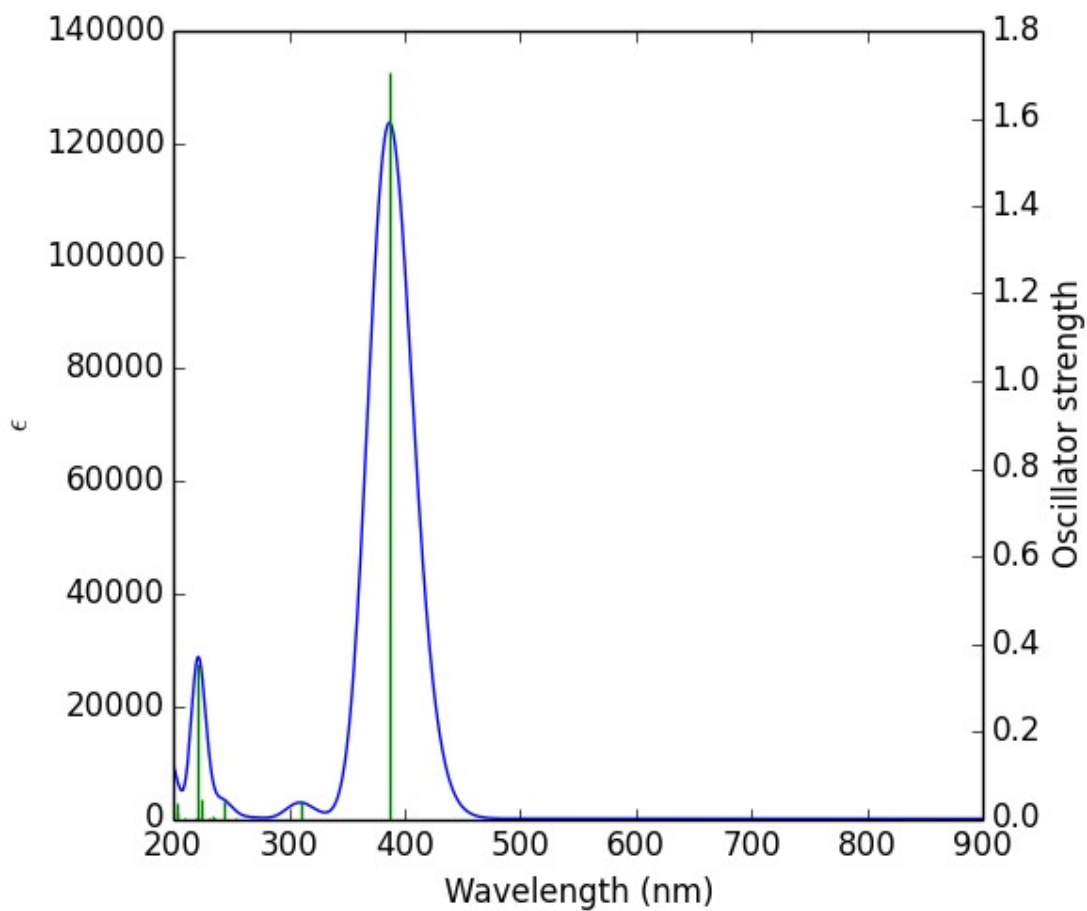


Figure S57. The computed absorption spectrum of Boc-*L*-Phe-TCF-1.

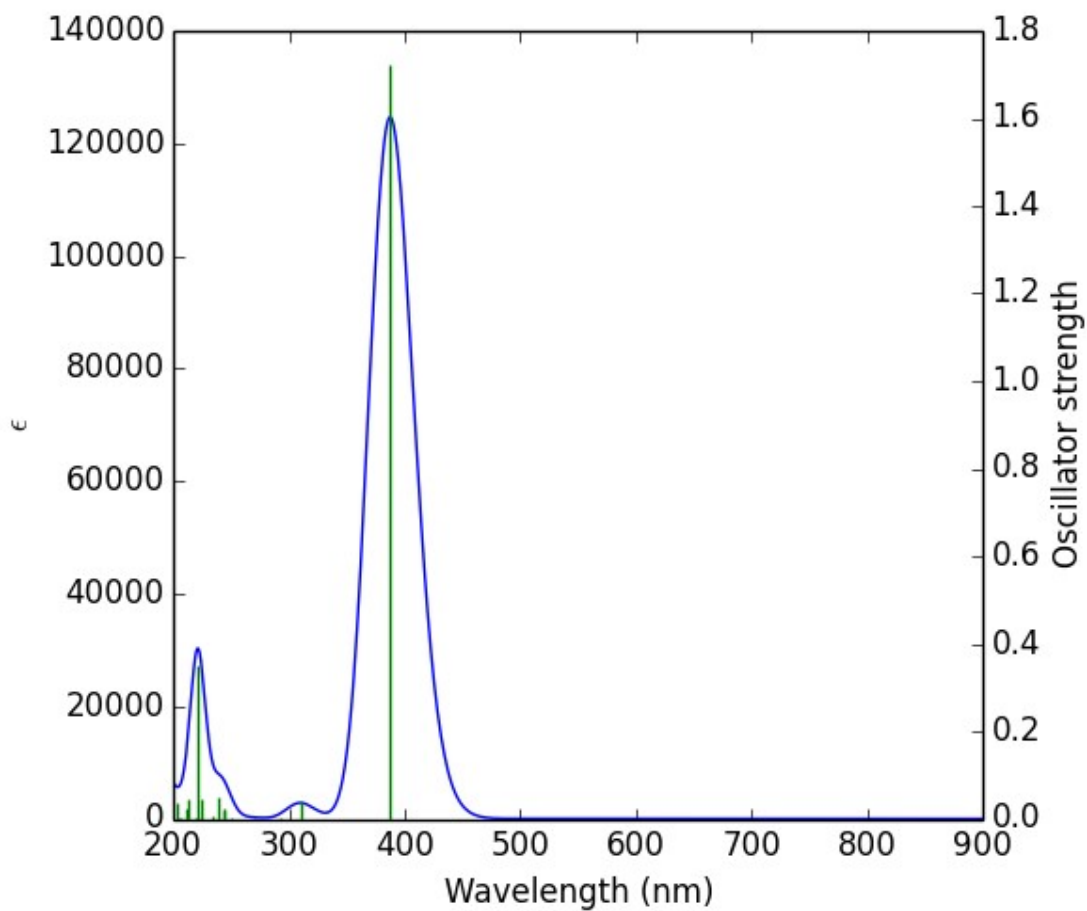


Figure S58. The computed absorption spectrum of Boc-*L*-tyr-TCF-1.

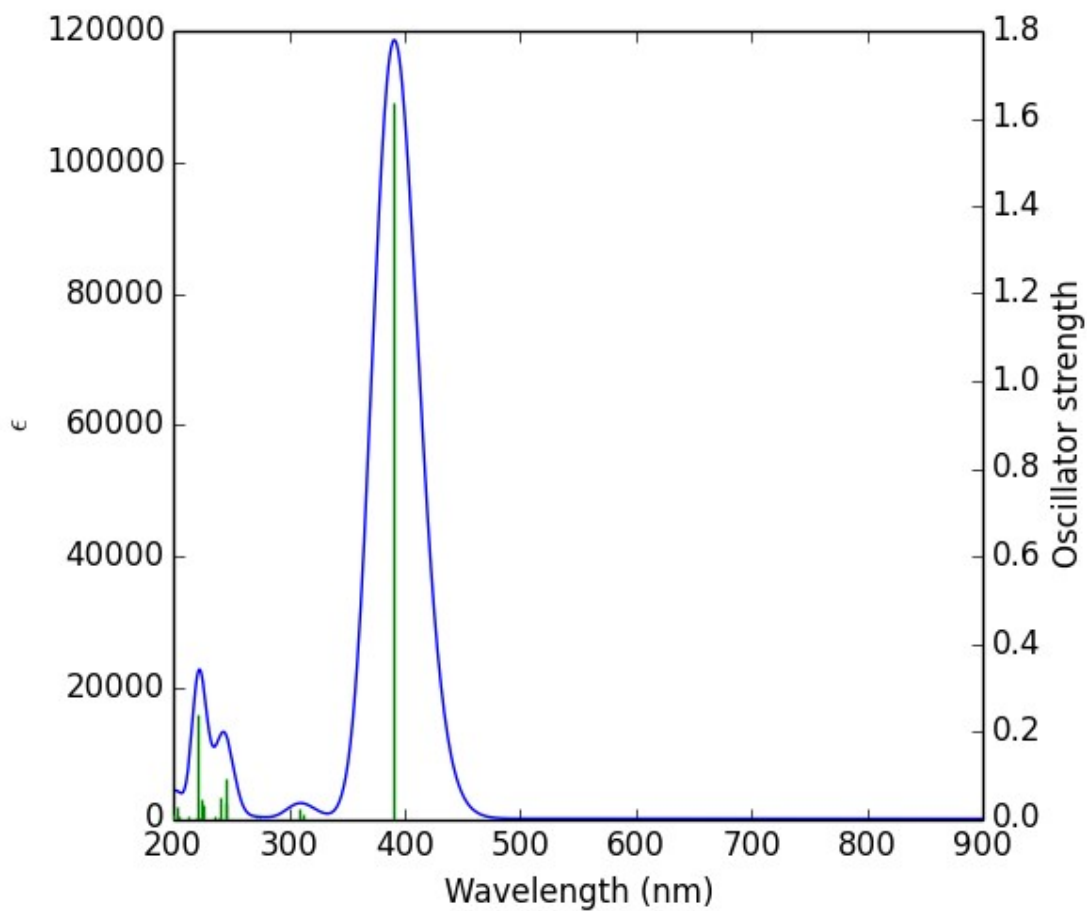


Figure S59. The computed absorption spectrum of Boc-L-Trp-TCF-1.

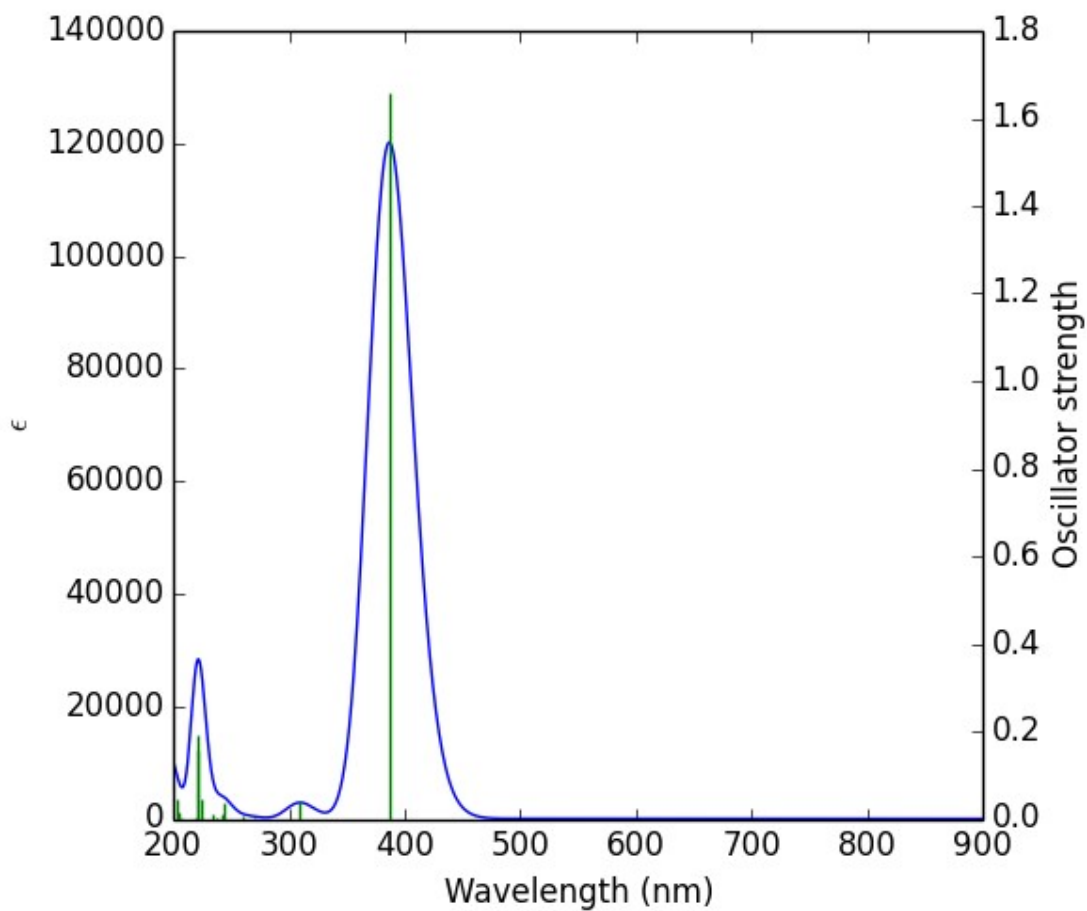


Figure S60. The computed absorption spectrum of L-Phe-TCF-1.

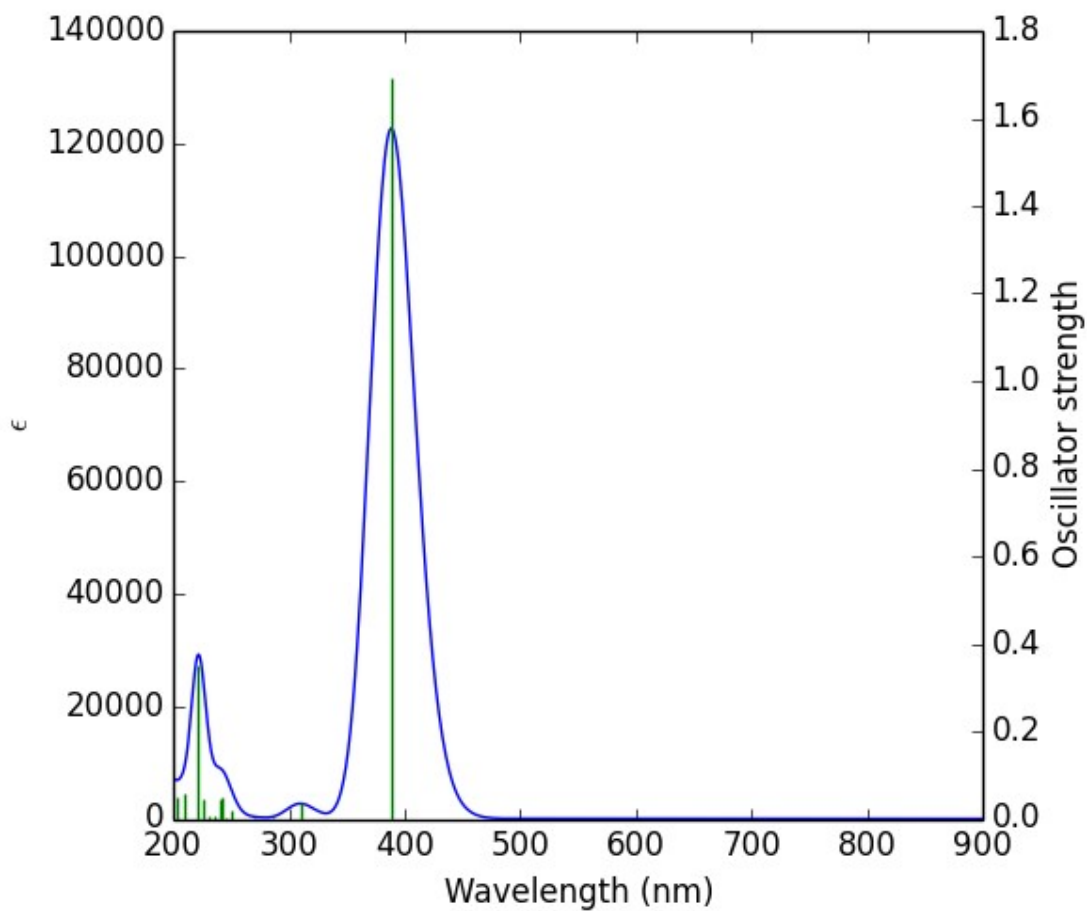


Figure S61. The computed absorption spectrum of *L*-Tyr-TCF-1.

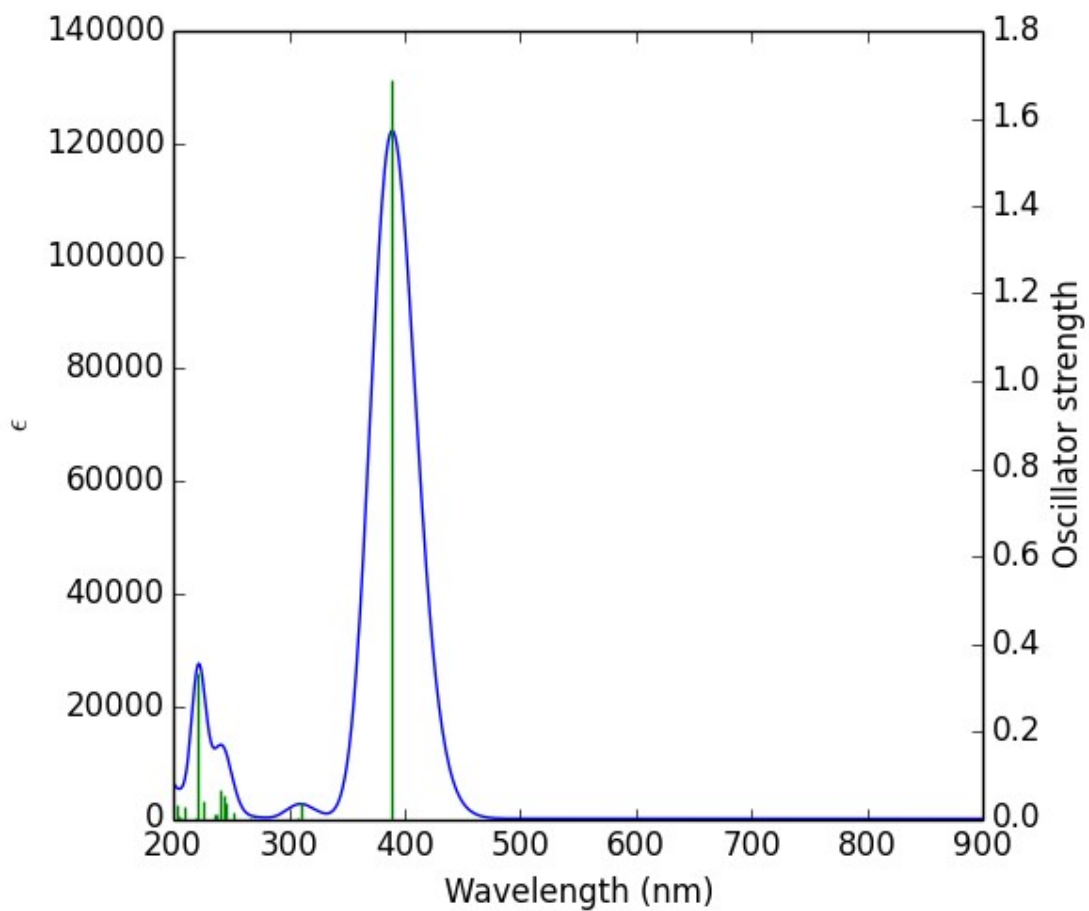


Figure S62. The computed absorption spectrum of *L*-Trp-TCF-1.