

Supplementary materials for

Structural optimization and structure–activity relationship of 4-thiazolidinone derivatives as novel inhibitors of human dihydroorotate dehydrogenase

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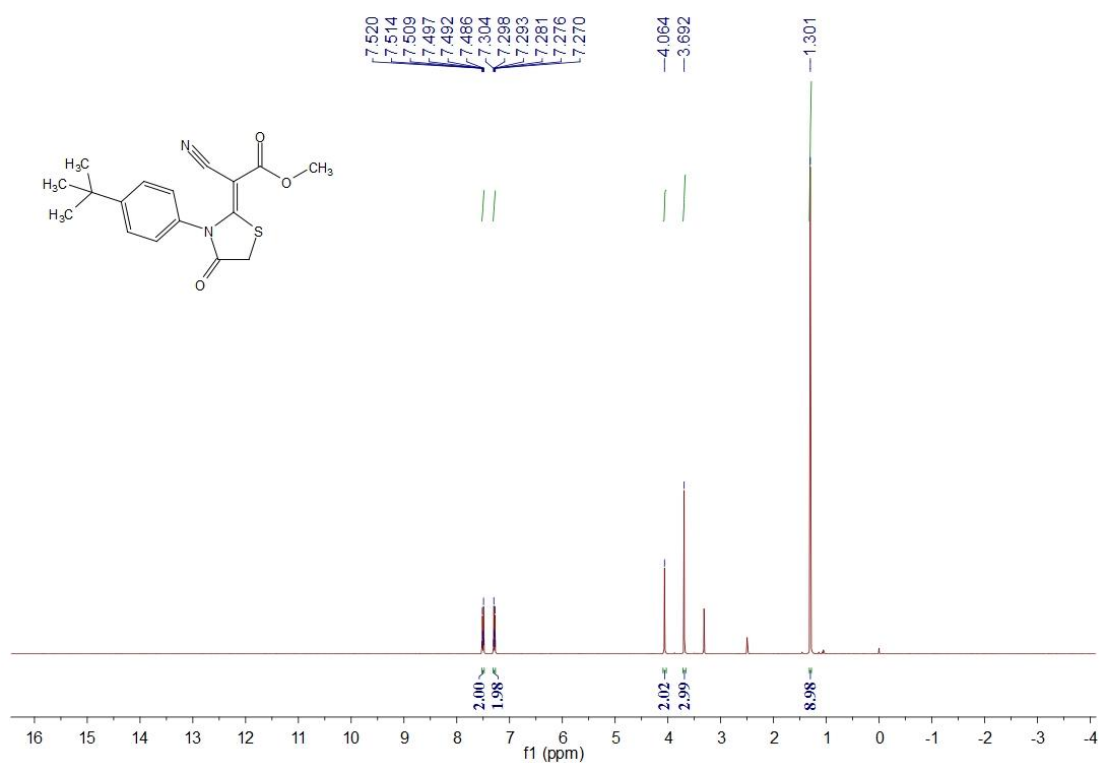
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1. Shanghai Key Laboratory of Chemical Biology, School of Pharmacy, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, PR China, xyxu@ecust.edu.cn (X.X.); Tel.: +86-21-64252945 (X.X.);

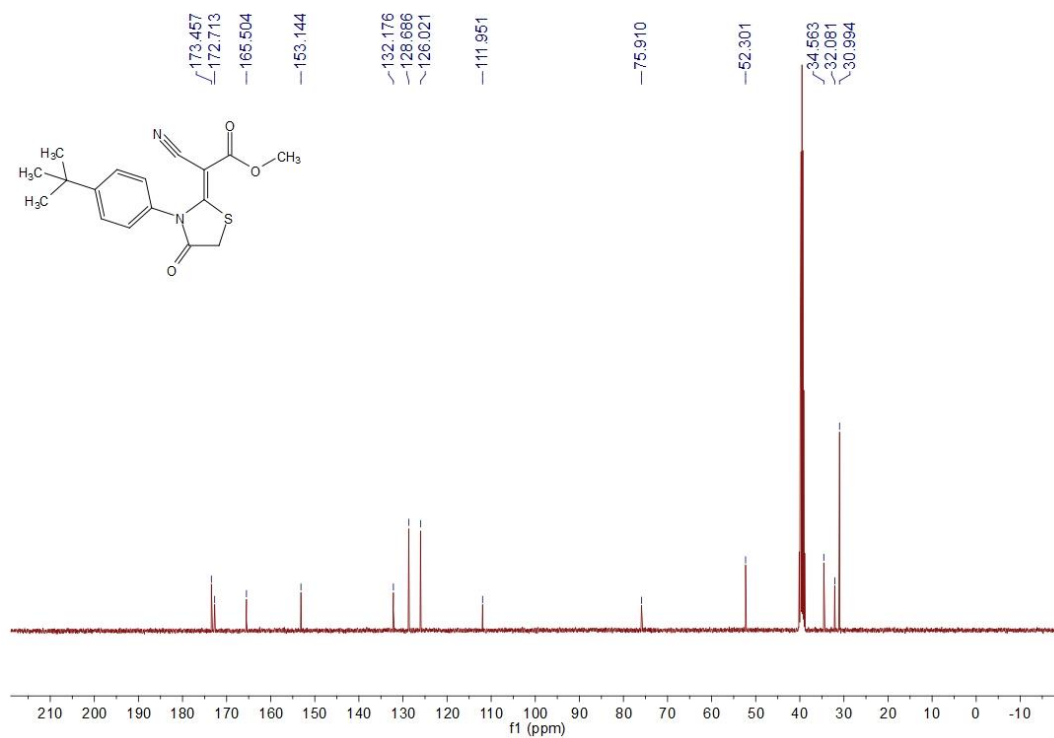
2. Shanghai Key Laboratory of New Drug Design, State Key Laboratory of Bioreactor Engineering, School of Pharmacy, East China University of Science & Technology, Shanghai 200237, PR China zhulfl@ecust.edu.cn (L.Z.); Tel.: +86-21-64253379 (L.Z.)

§ These authors contributed equally to this work.

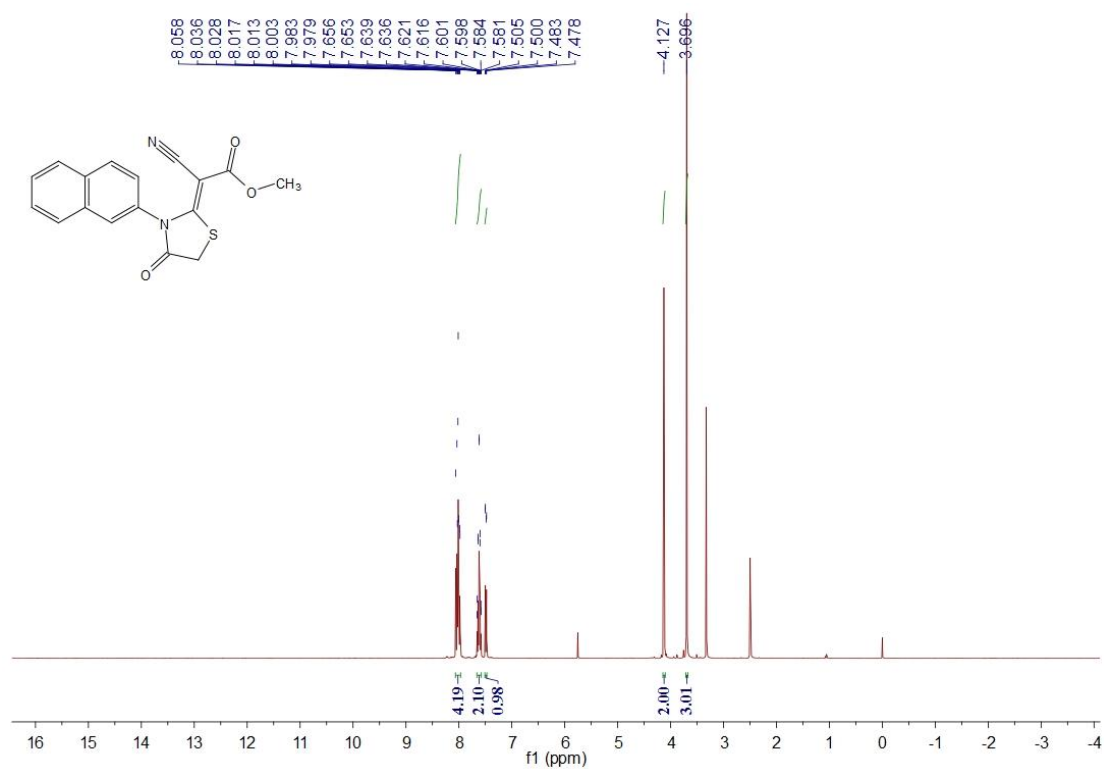
The copies of spectrum for target compounds 7-46. (^1H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded on Bruker AM-400 (^1H at 400 MHz, ^{13}C at 100 MHz, ^{19}F at 376 MHz) spectrometer with CDCl_3 or $\text{DMSO}-d_6$ as the solvent and TMS as the internal standard.)



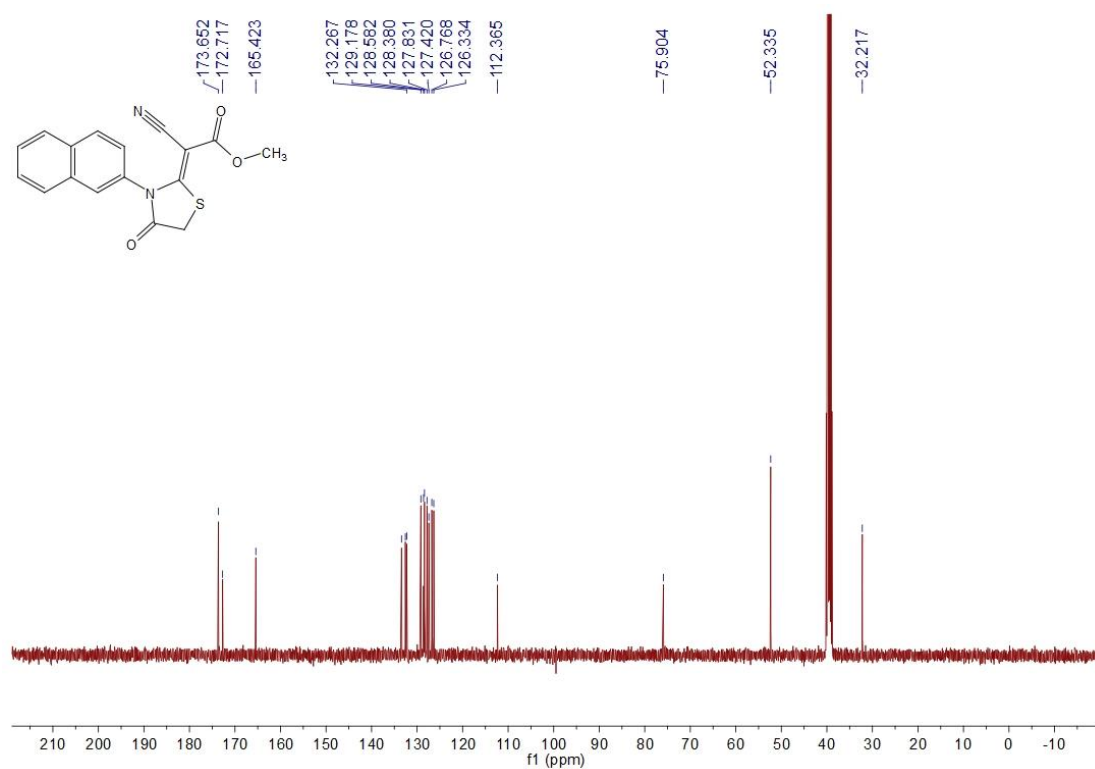
FigureS1. ^1H -NMR of compound 7.



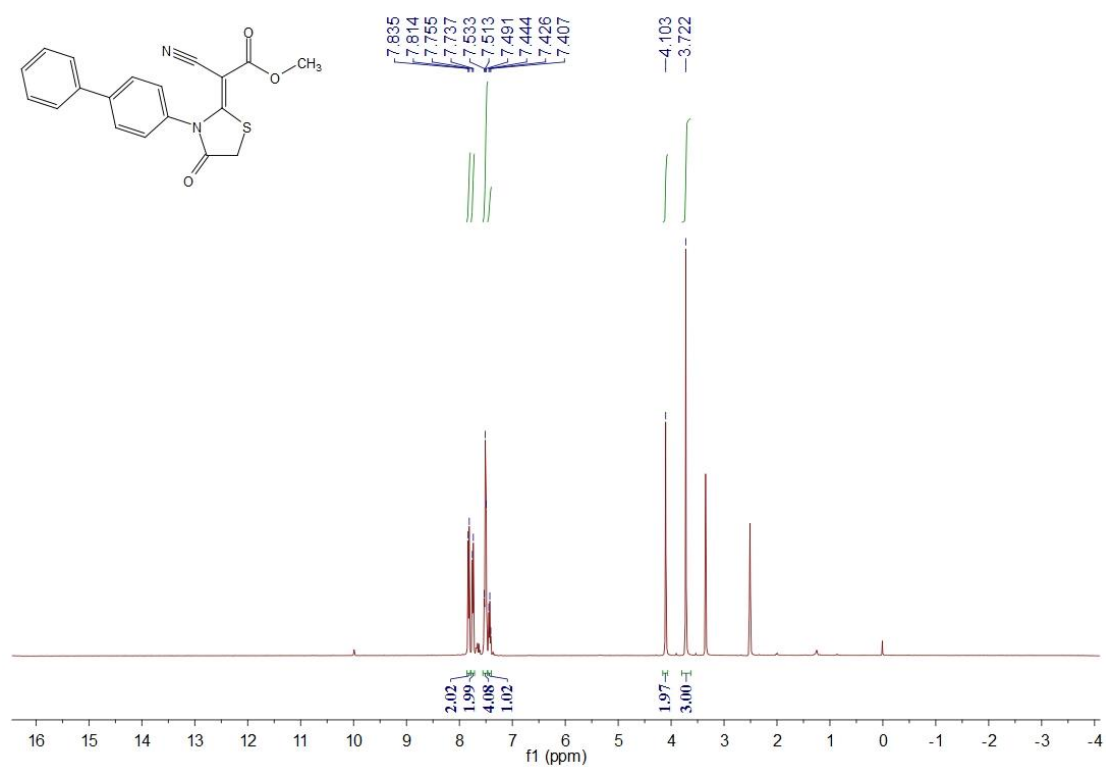
FigureS2. ^{13}C -NMR of compound 7.



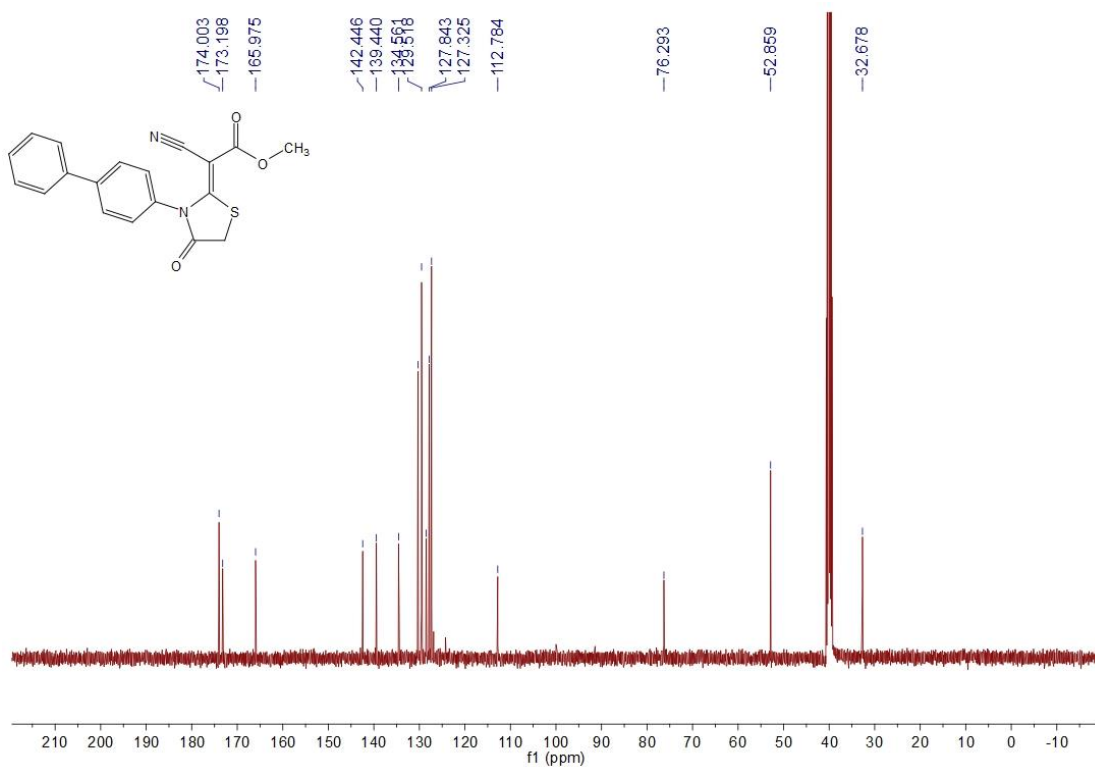
FigureS3. ¹H-NMR of compound 8.



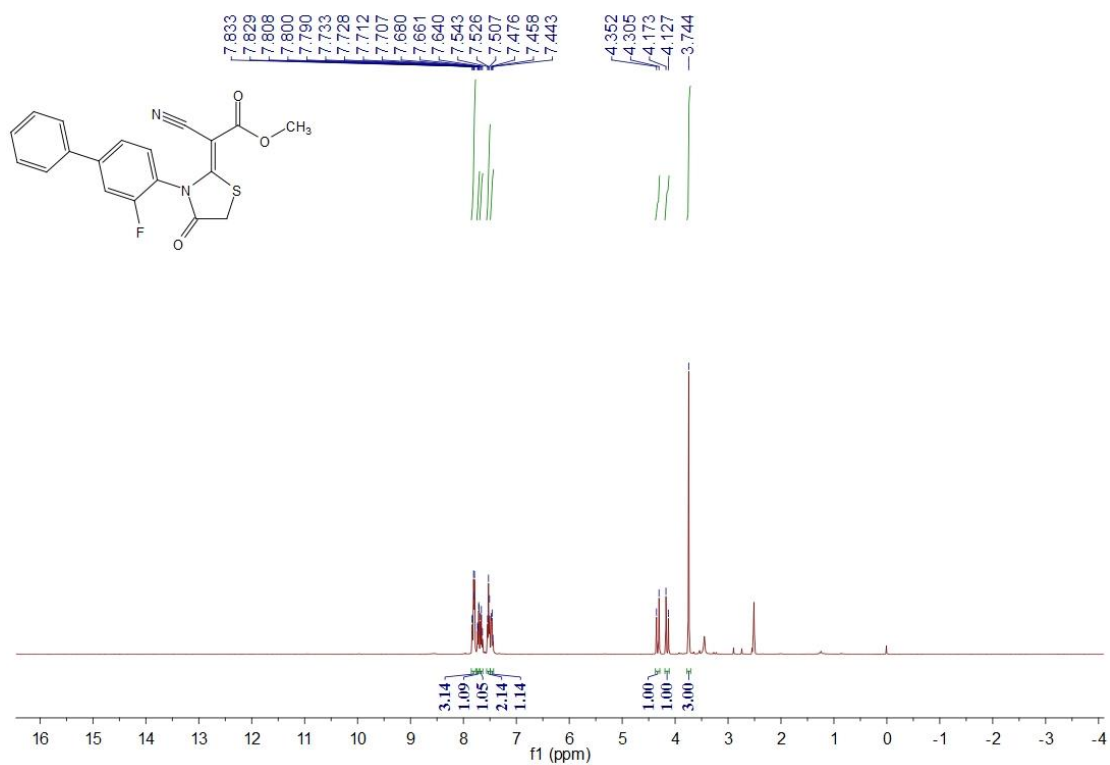
FigureS4. ¹³C-NMR of compound 8.



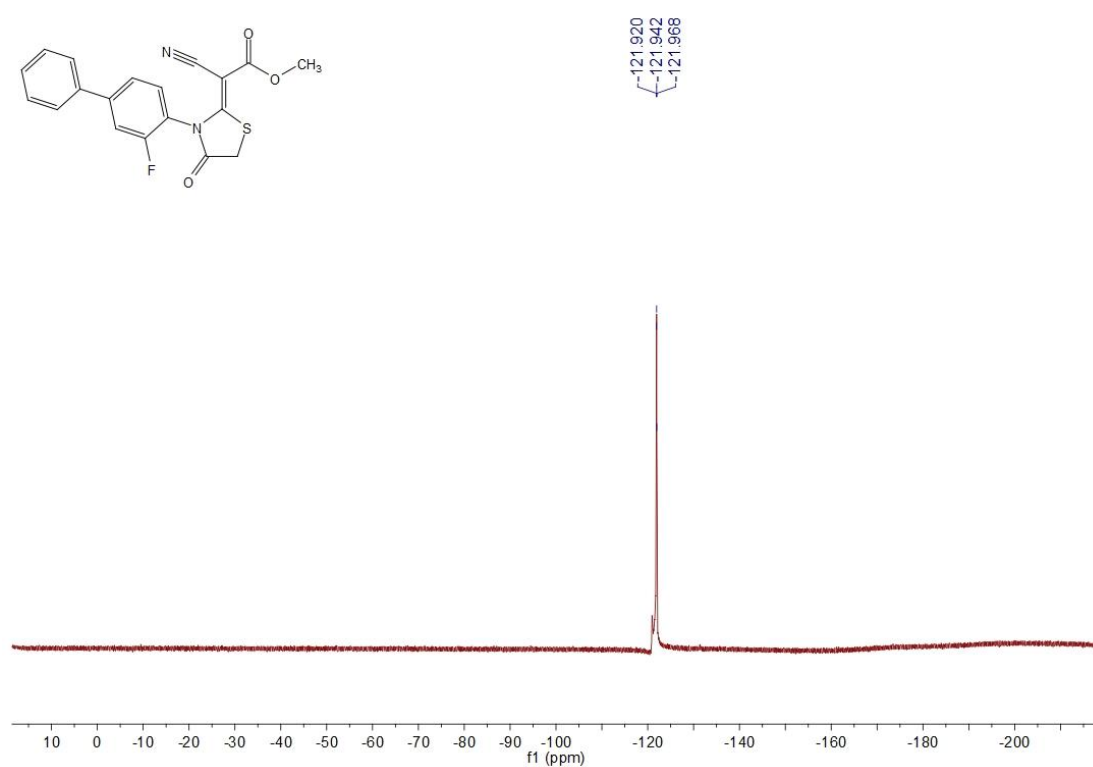
FigureS5. ¹H-NMR of compound 9.



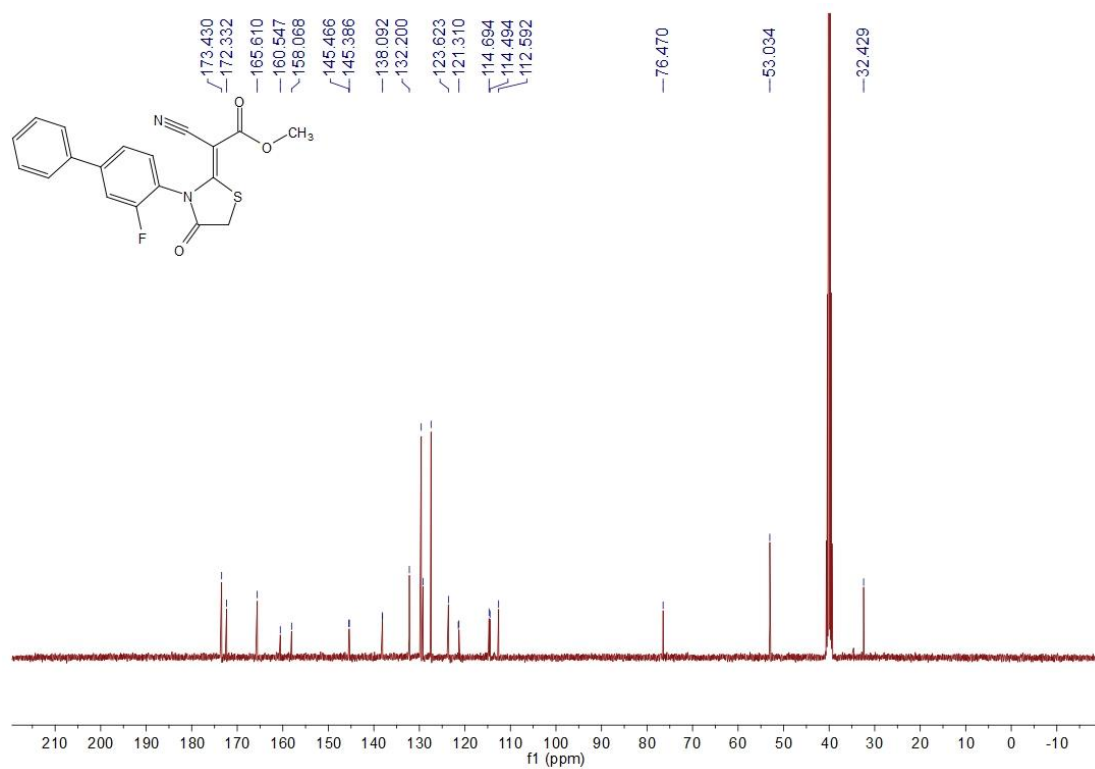
FigureS6. ¹³C-NMR of compound 9.



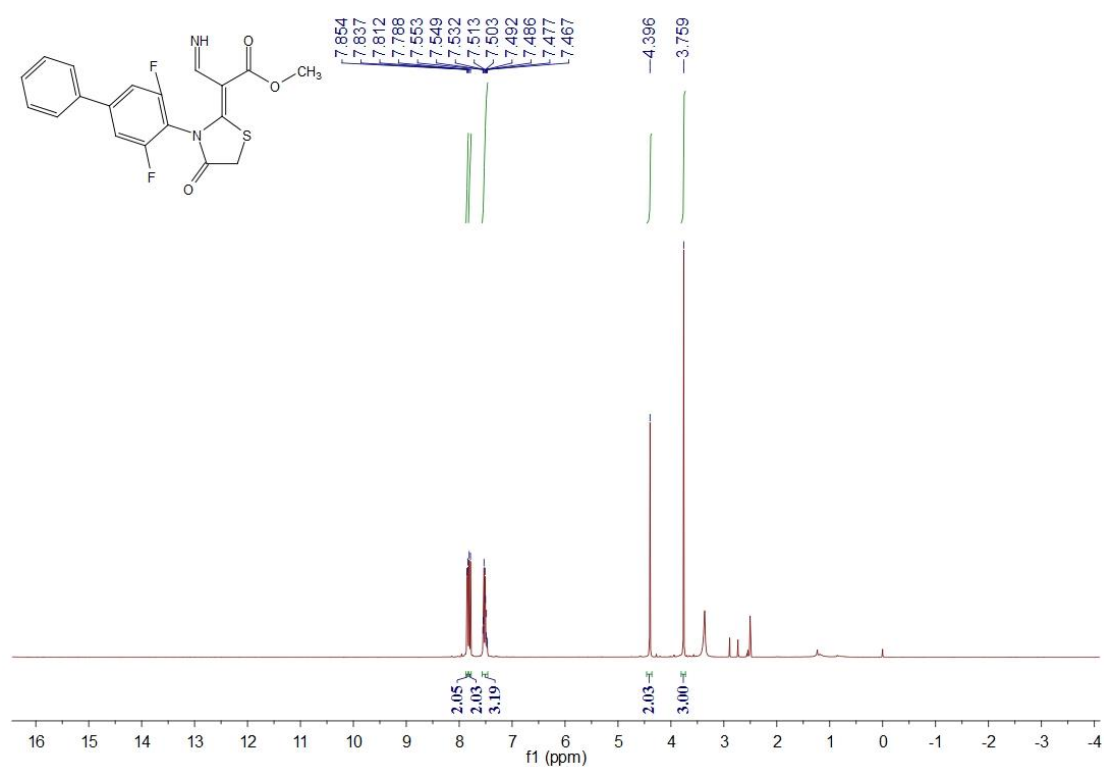
FigureS7. ¹H-NMR of compound 10.



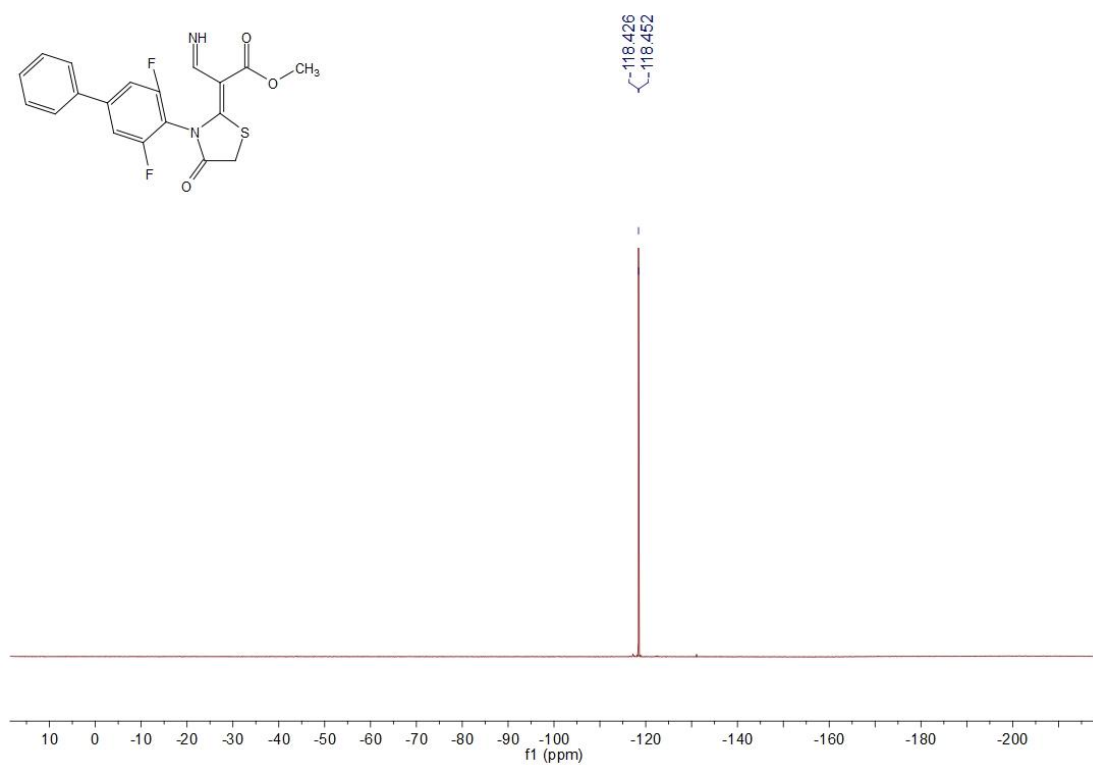
FigureS8. ¹⁹F-NMR of compound 10.



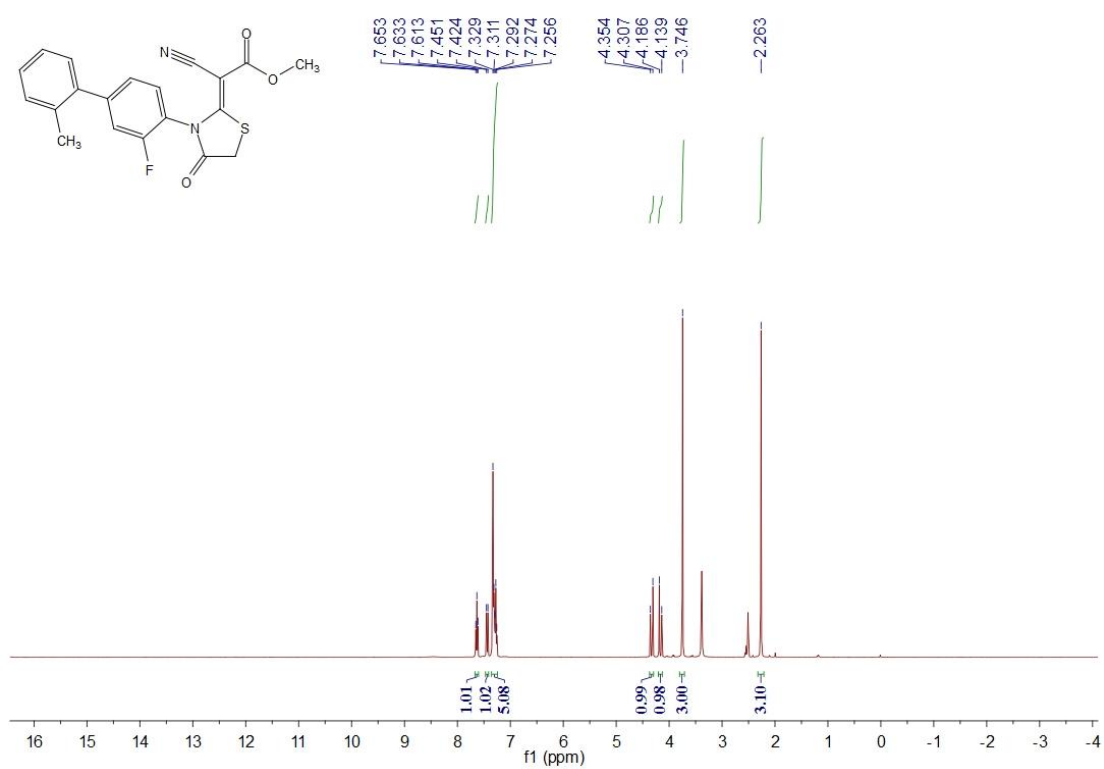
FigureS9. ¹³C-NMR of compound 10.



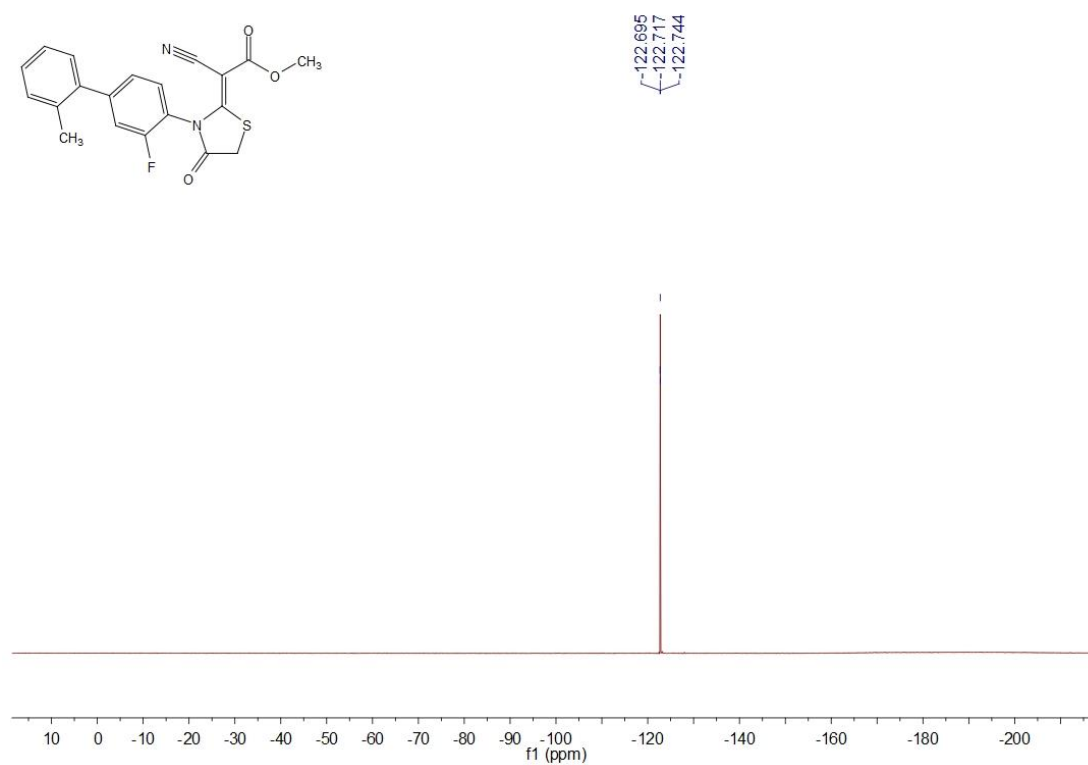
FigureS10. ¹H-NMR of compound 11.



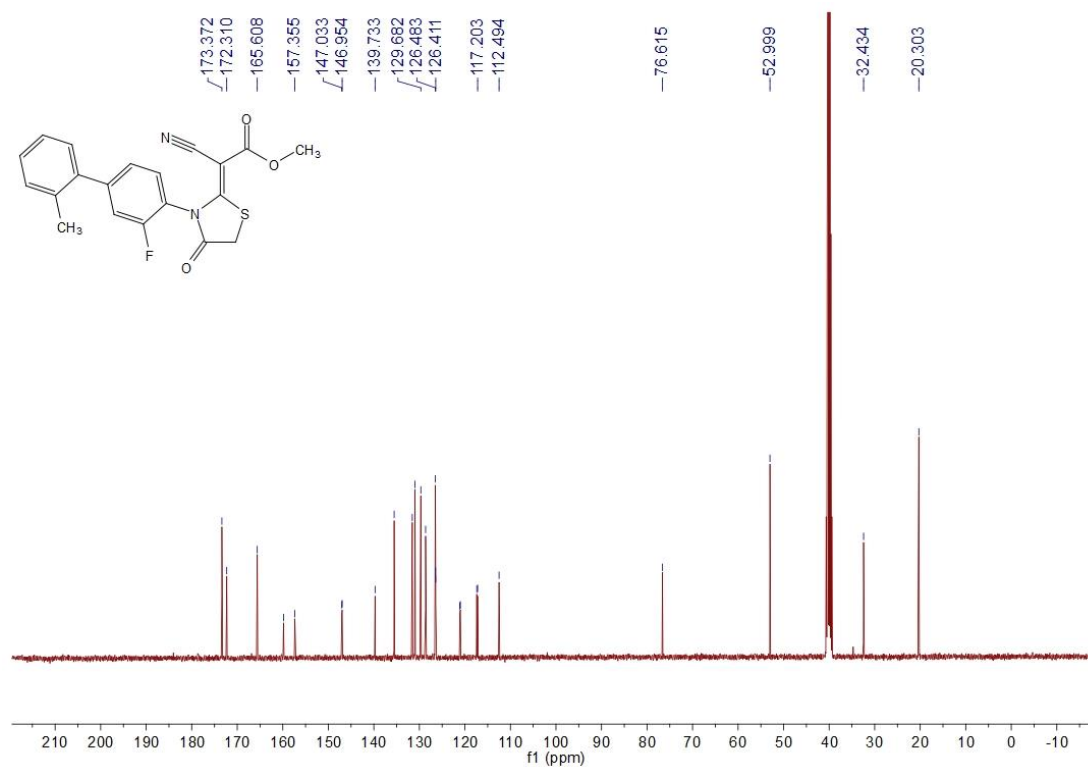
FigureS11. ^{19}F -NMR of compound 11.



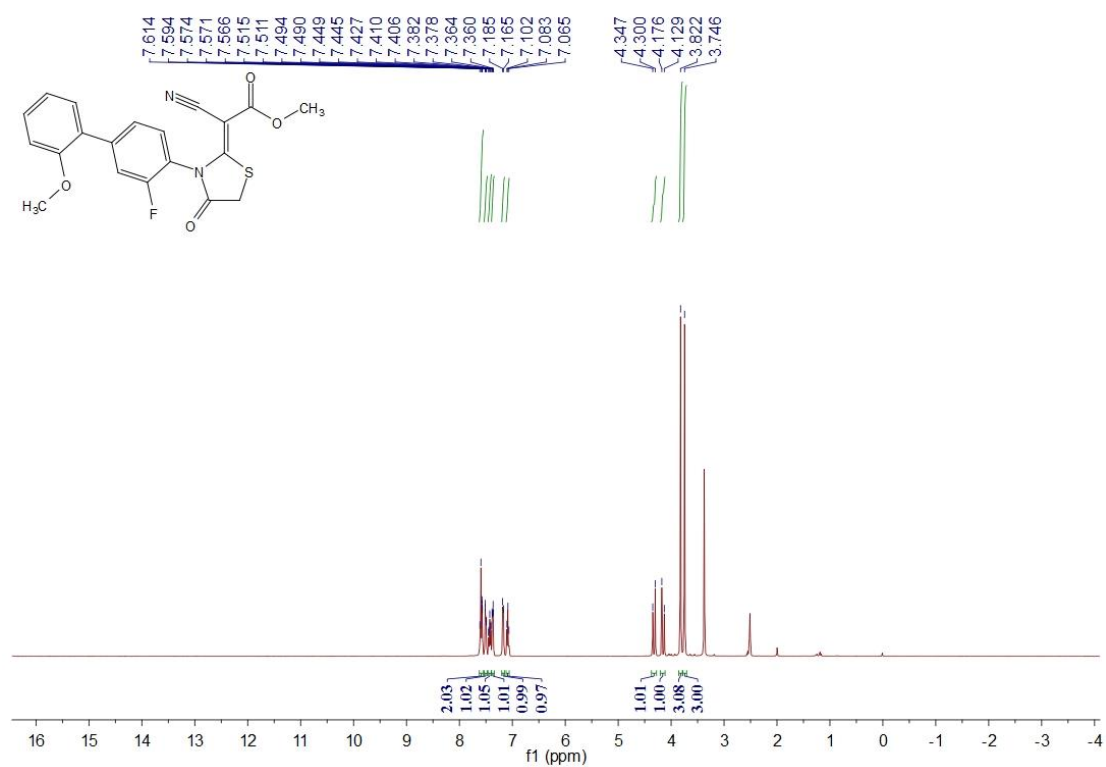
FigureS12. ^1H -NMR of compound 12.



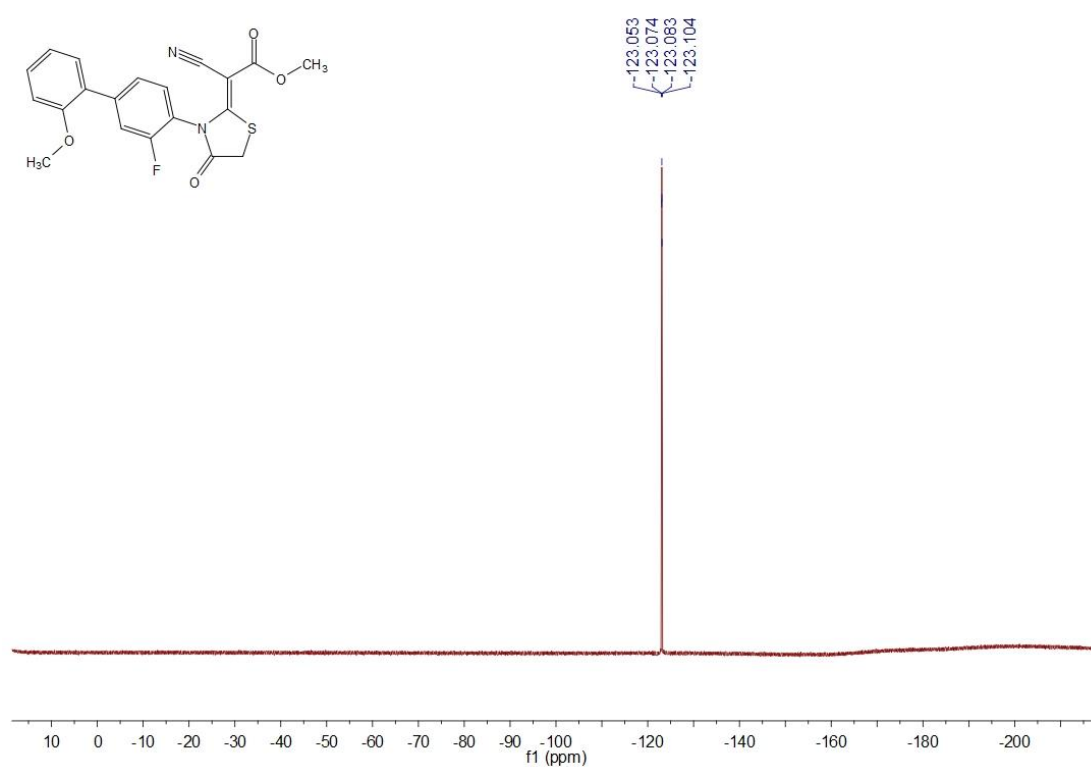
FigureS13. ¹⁹F-NMR of compound 12.



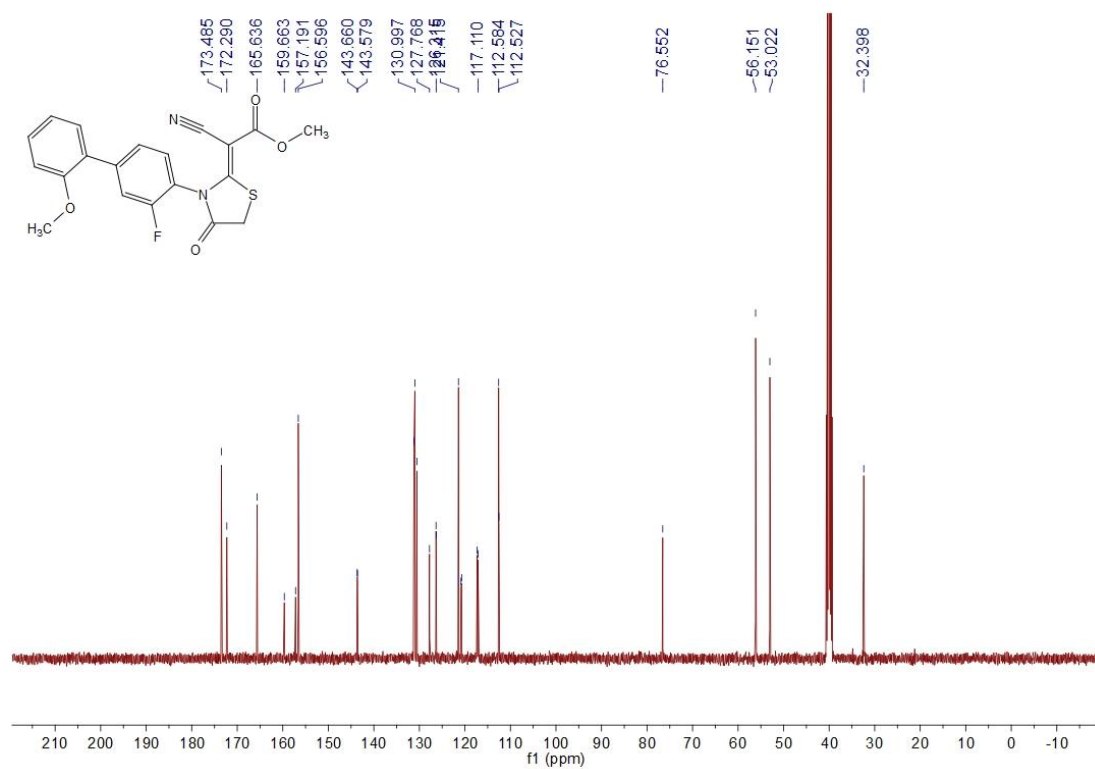
FigureS14. ¹³C-NMR of compound 12.



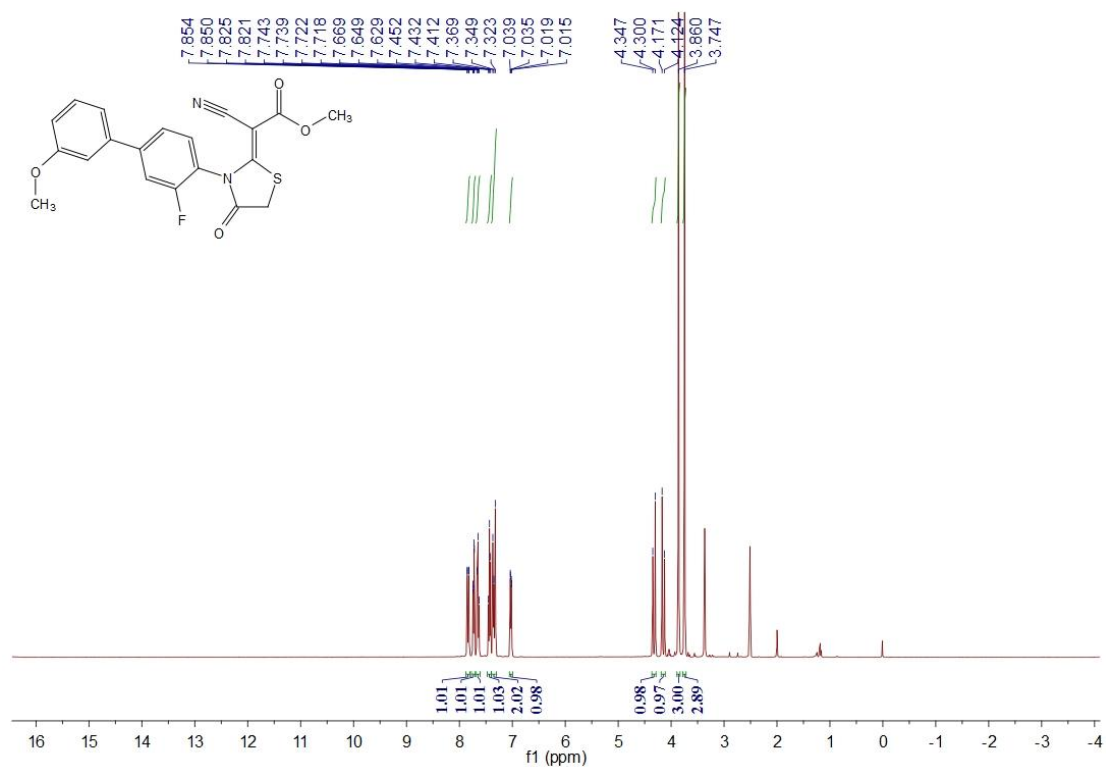
FigureS15. ¹H-NMR of compound 13.



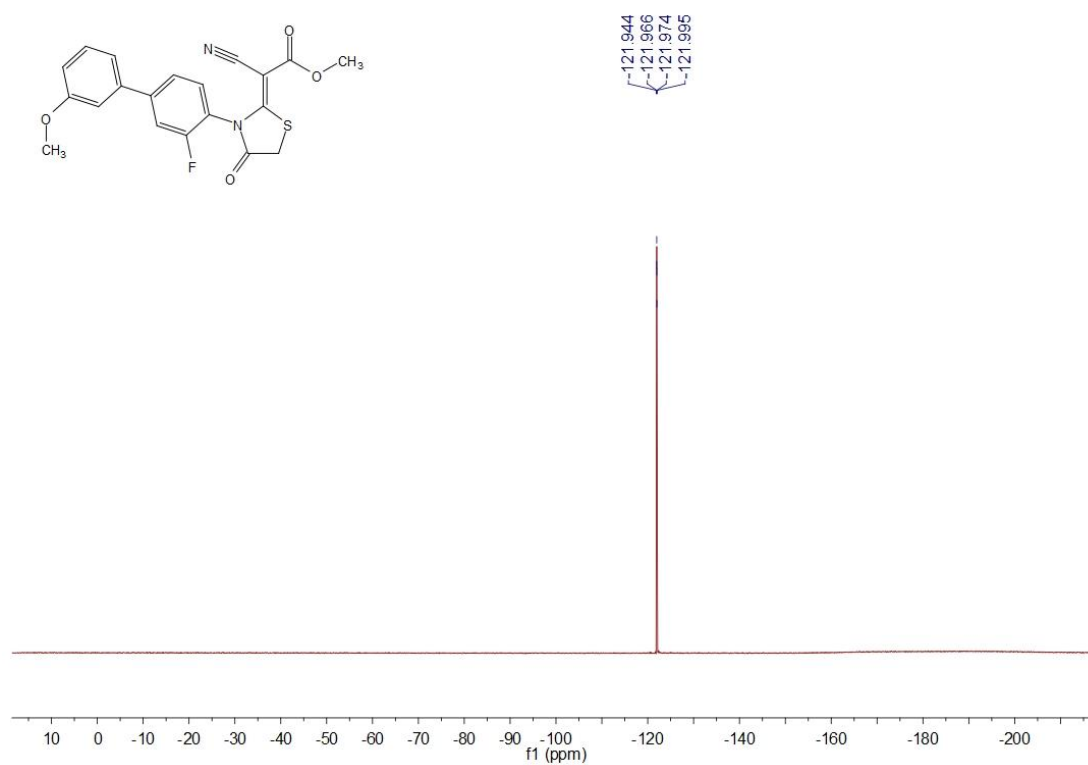
FigureS16. ¹⁹F-NMR of compound 13.



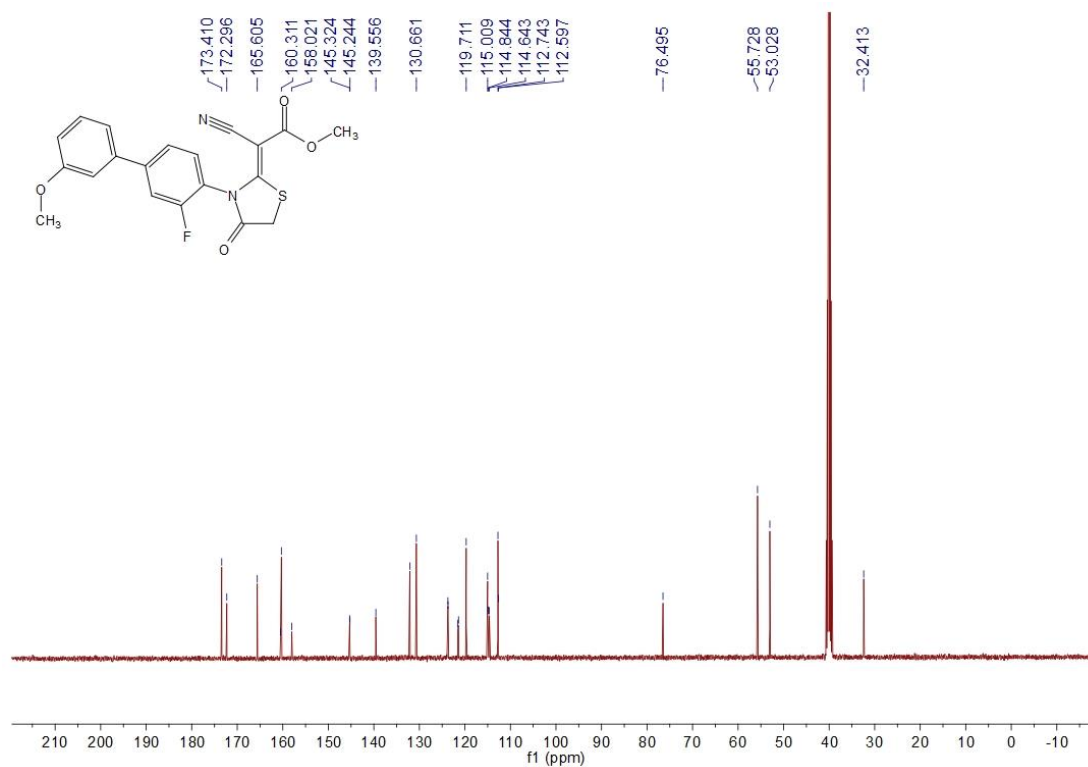
FigureS17. ¹³C-NMR of compound 13.



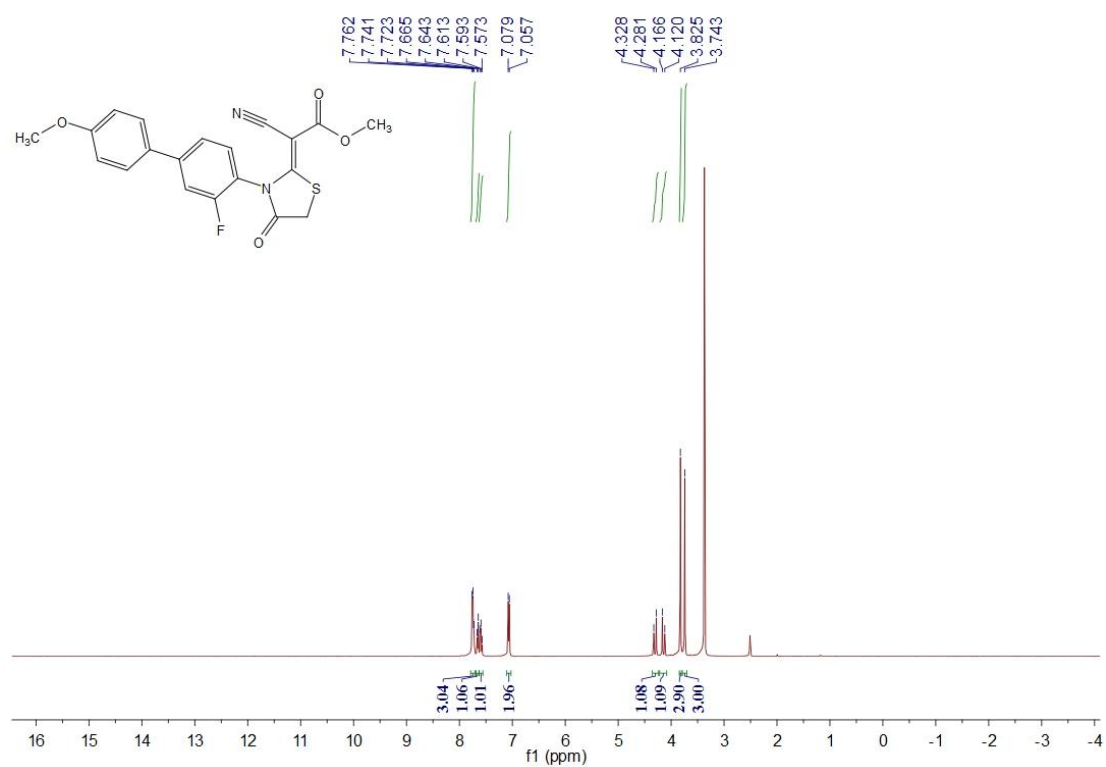
FigureS18. ¹H-NMR of compound 14.



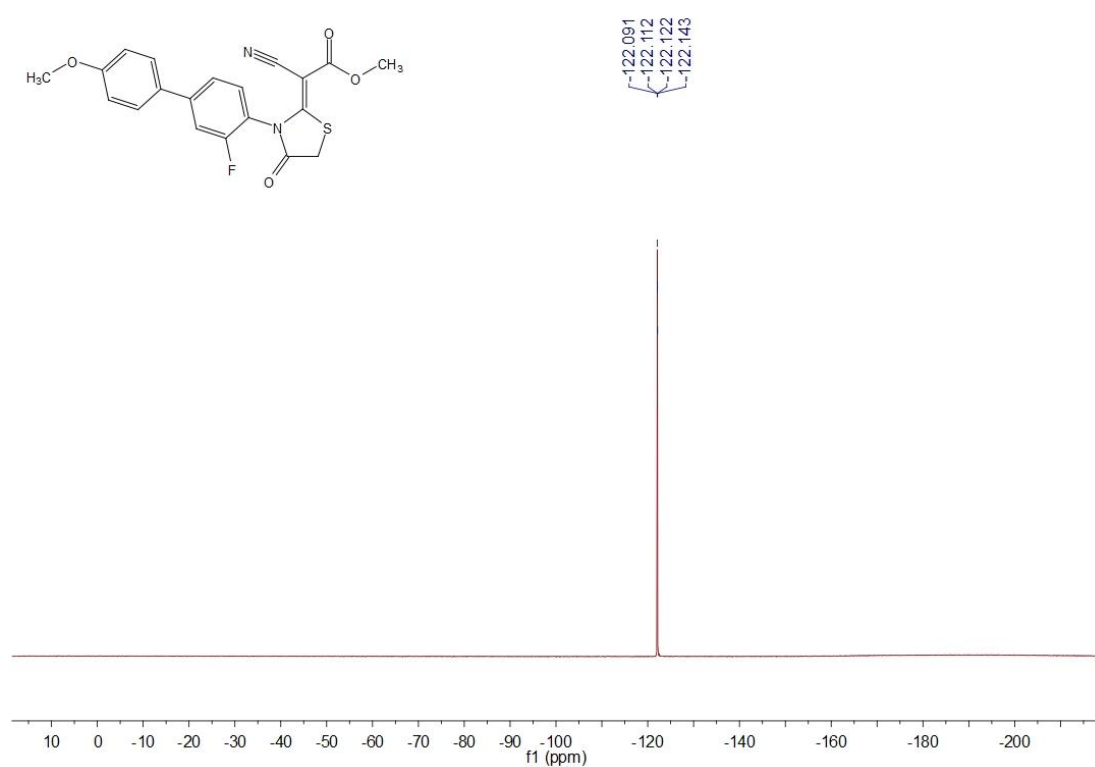
FigureS19. ¹⁹F-NMR of compound 14.



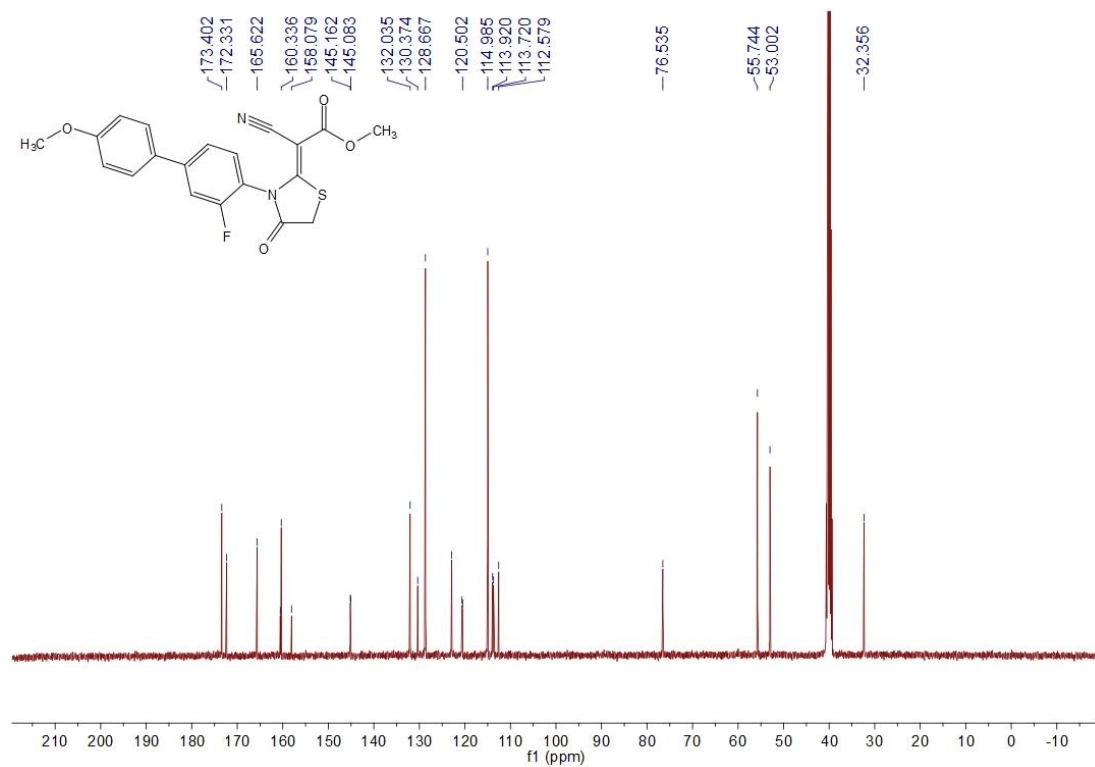
FigureS20. ¹³C-NMR of compound 14.



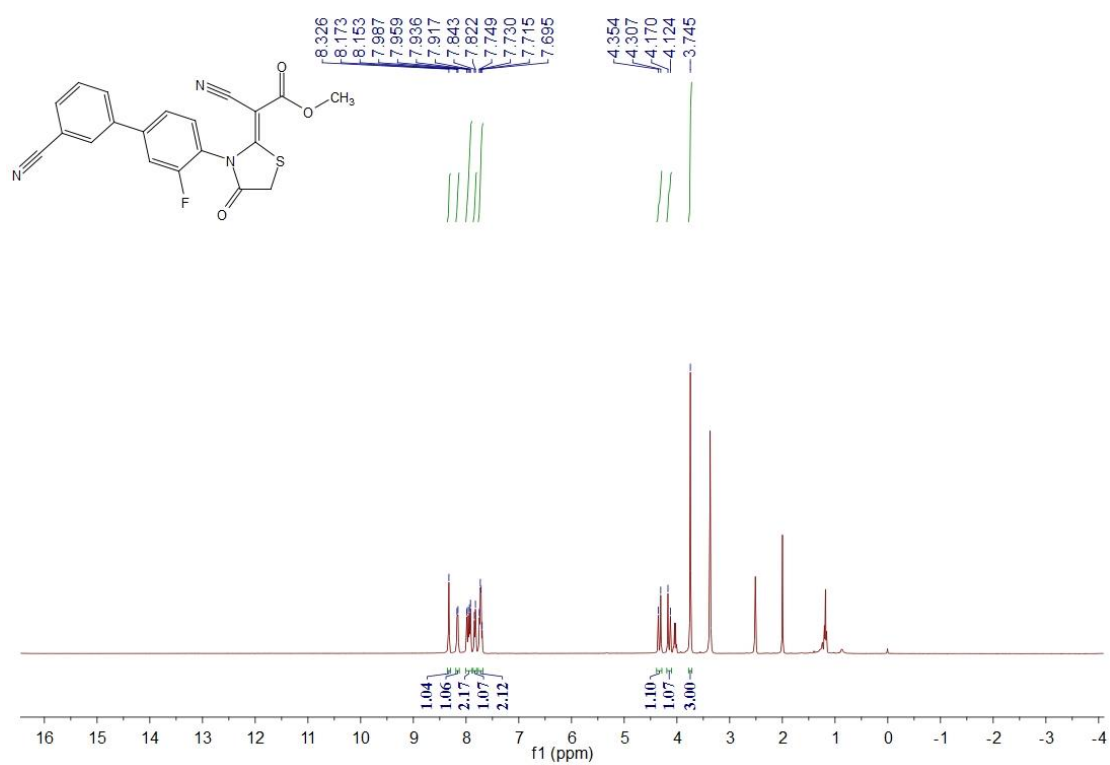
FigureS21.¹H-NMR of compound 15



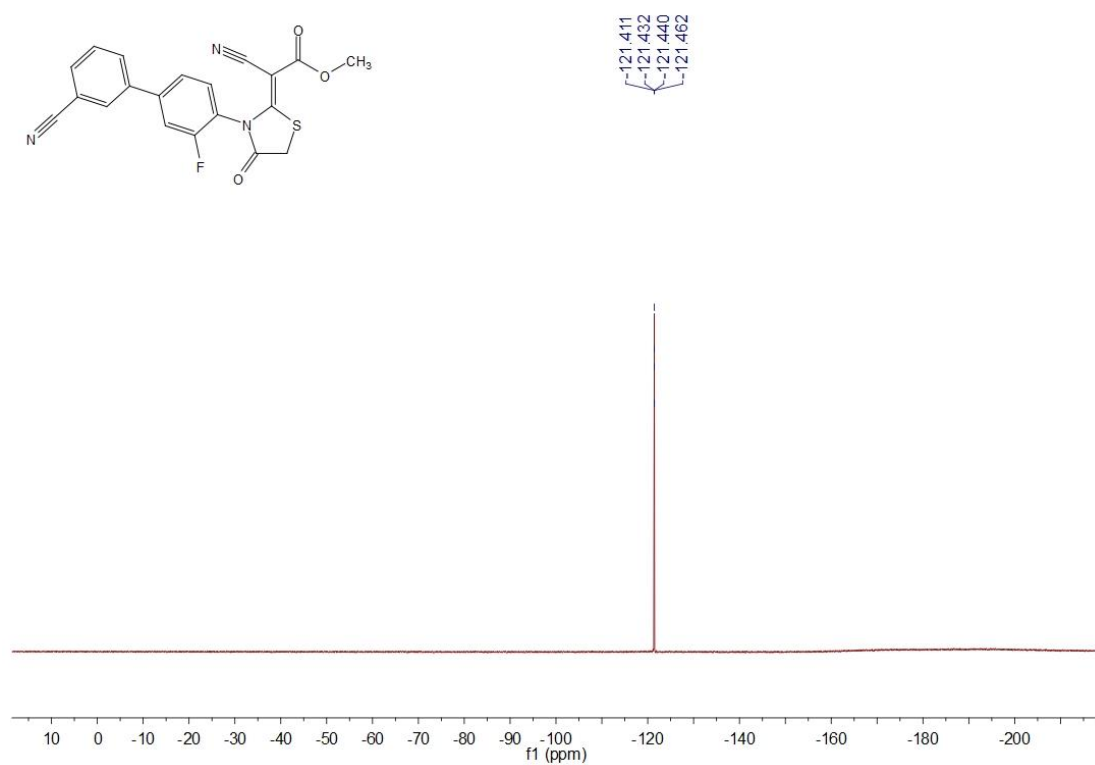
FigureS22.¹⁹F-NMR of compound 15.



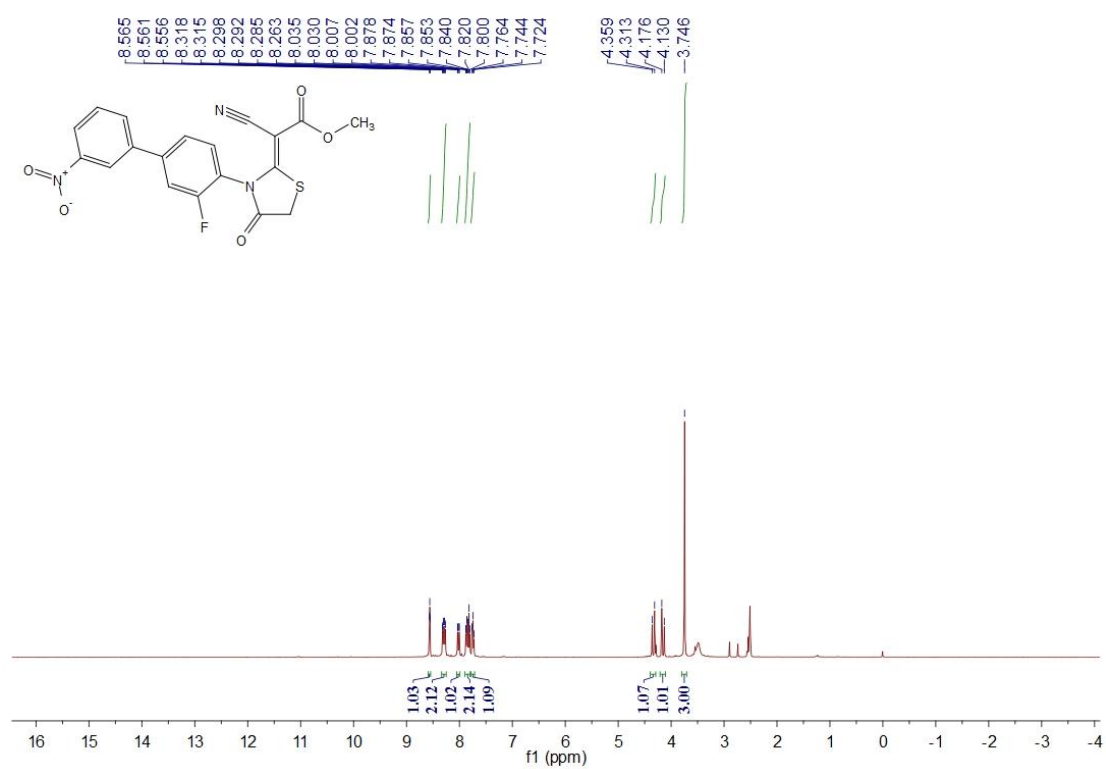
FigureS23. ¹³C-NMR of compound 15.



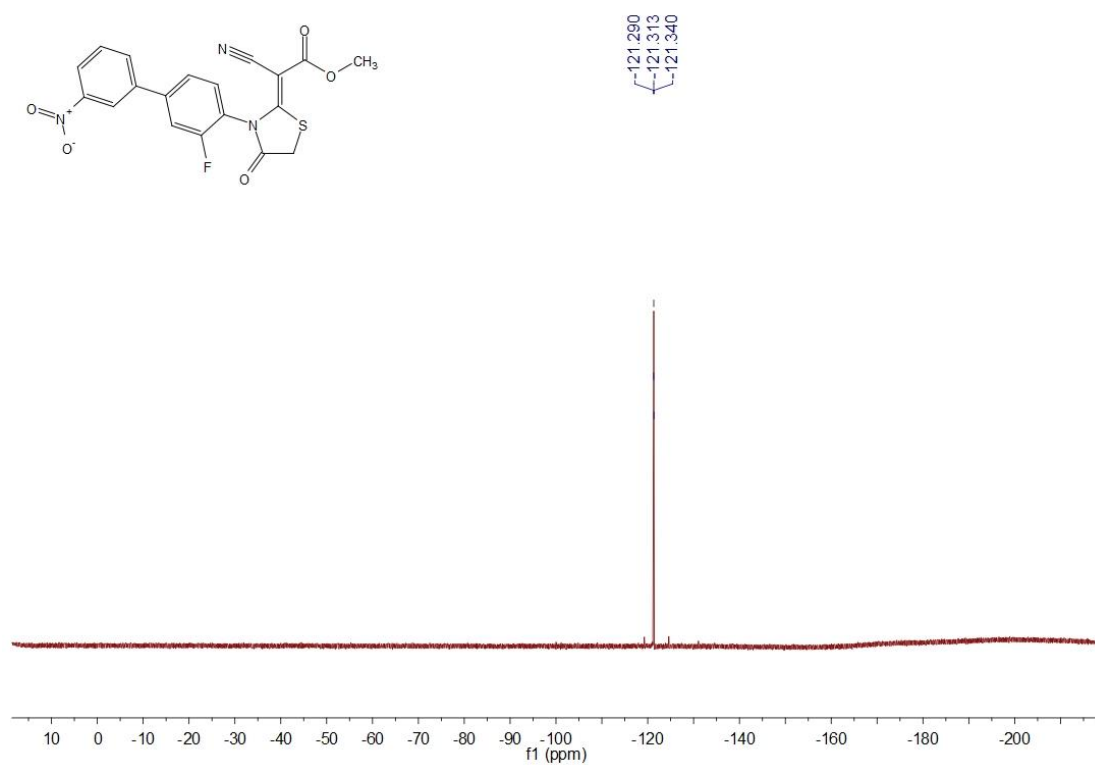
FigureS24. ¹H-NMR of compound 16.



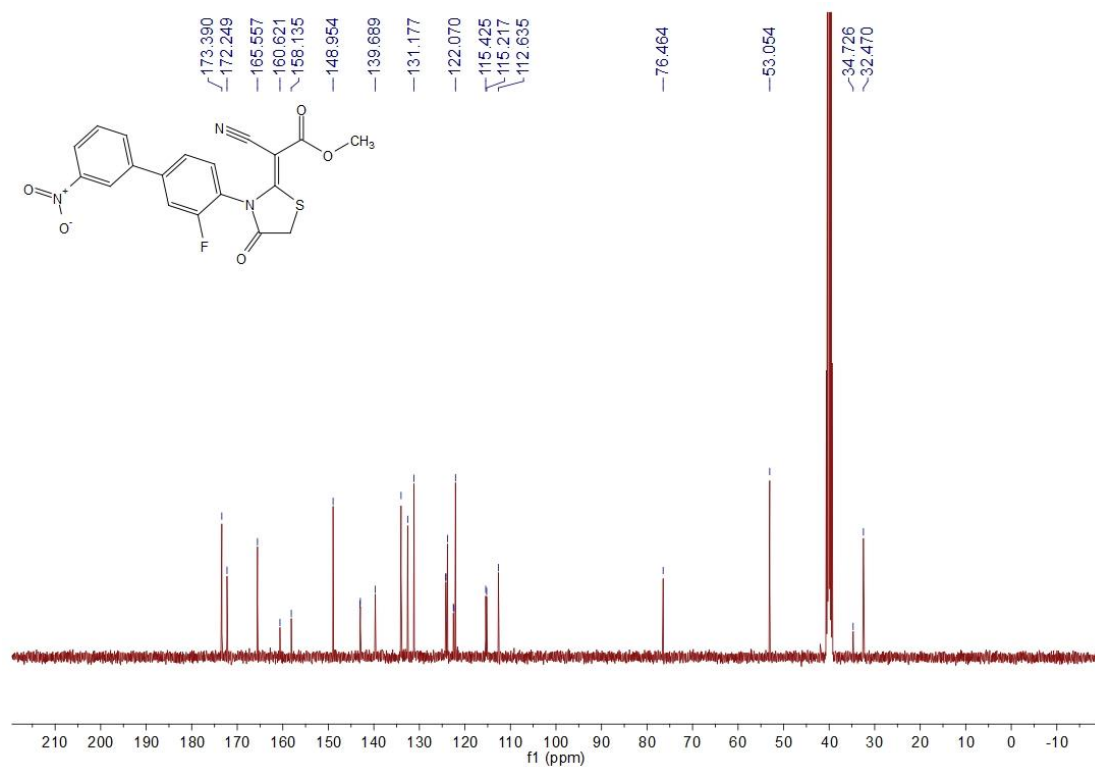
FigureS25. ¹⁹F-NMR of compound 16.



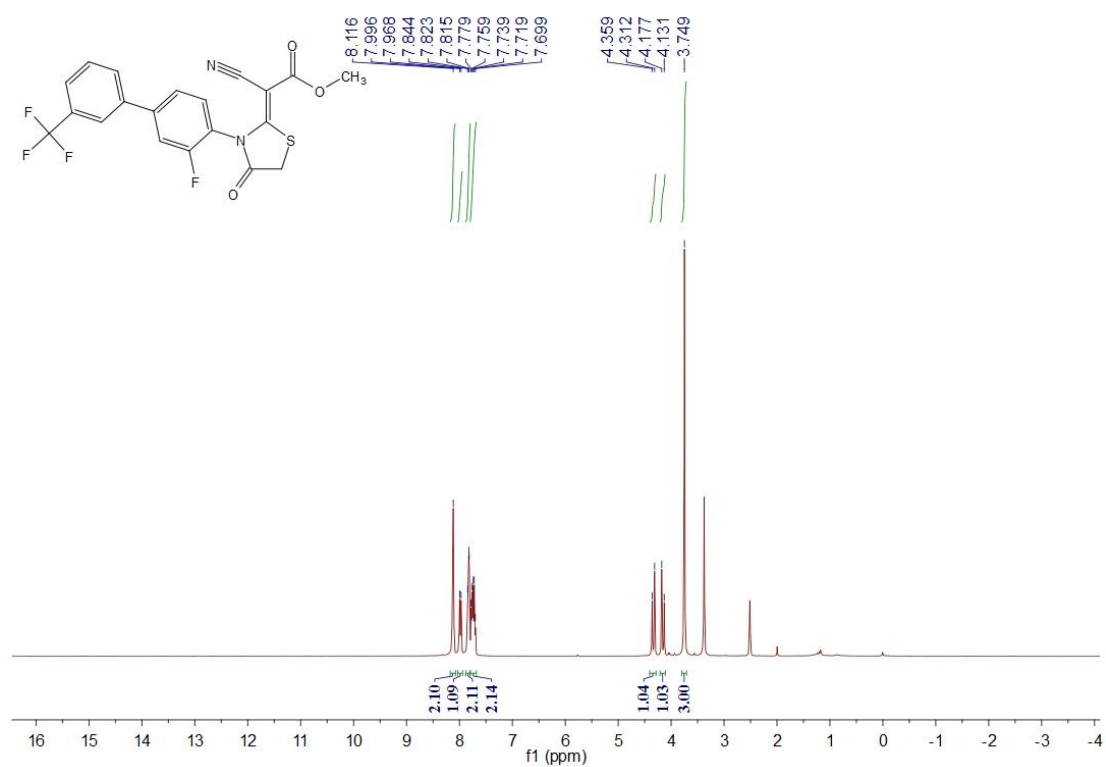
FigureS26. ¹H-NMR of compound 17.



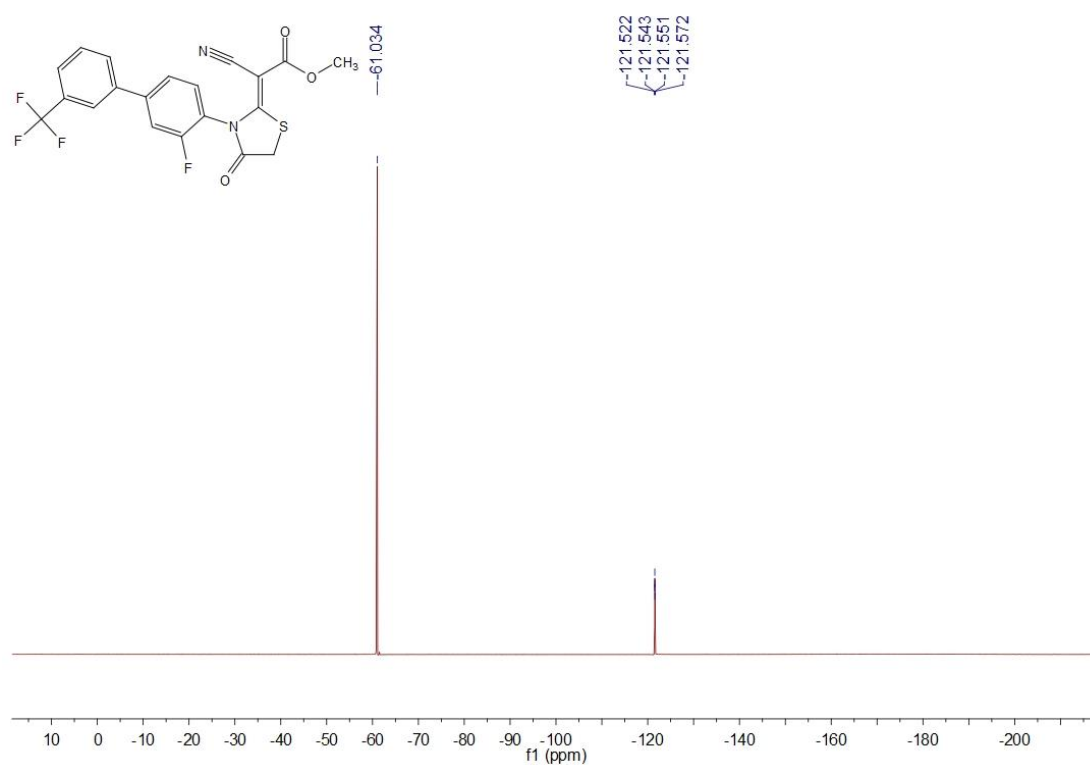
FigureS27. ¹⁹F-NMR of compound 17.



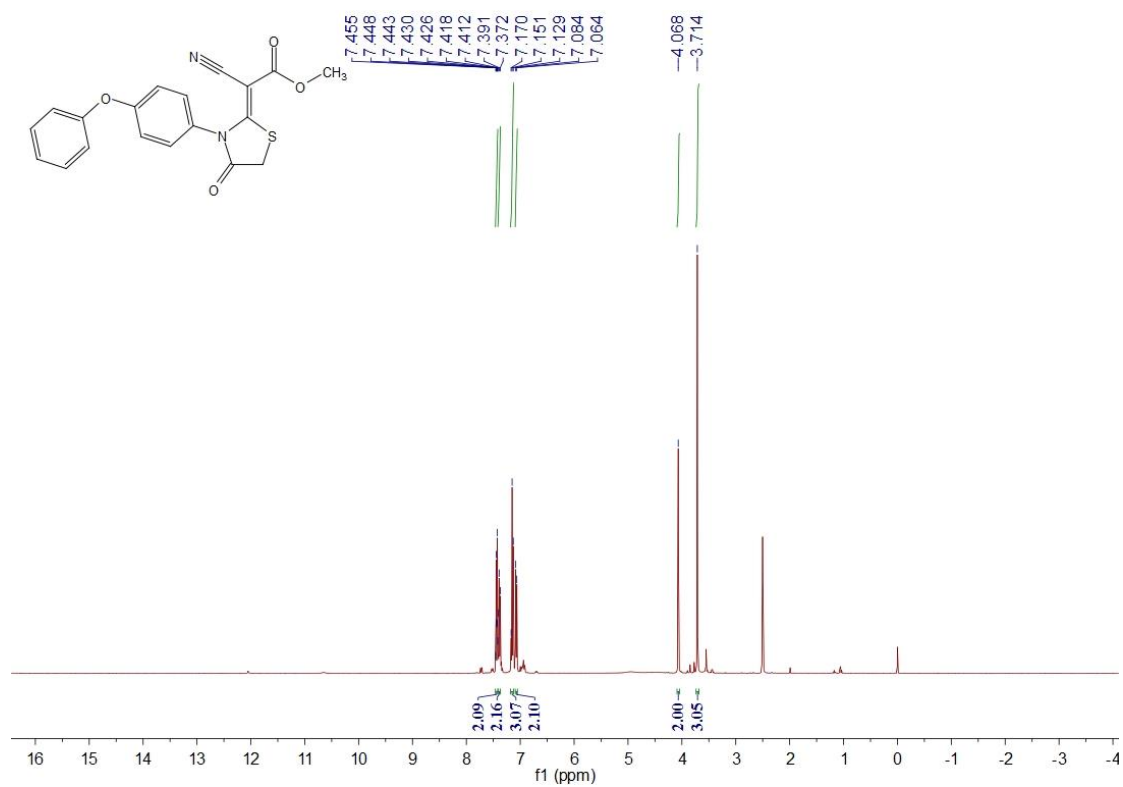
FigureS28. ¹³C-NMR of compound 17.



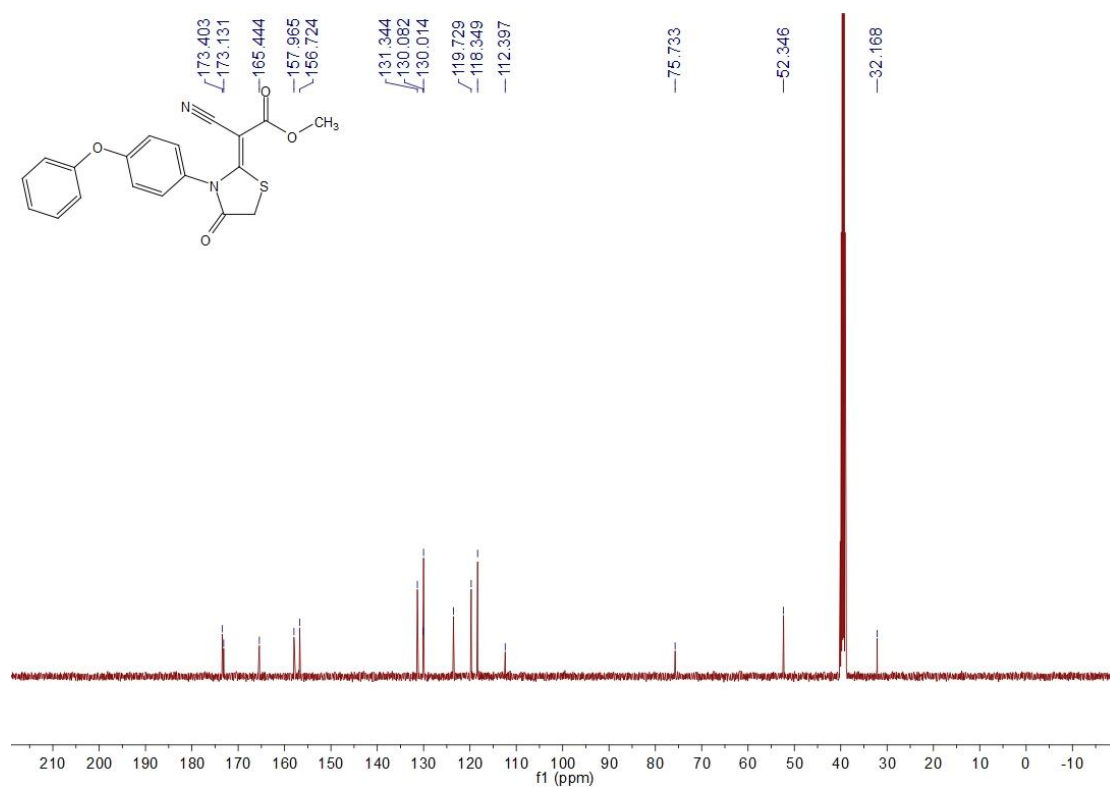
FigureS29.¹H-NMR of compound 18.



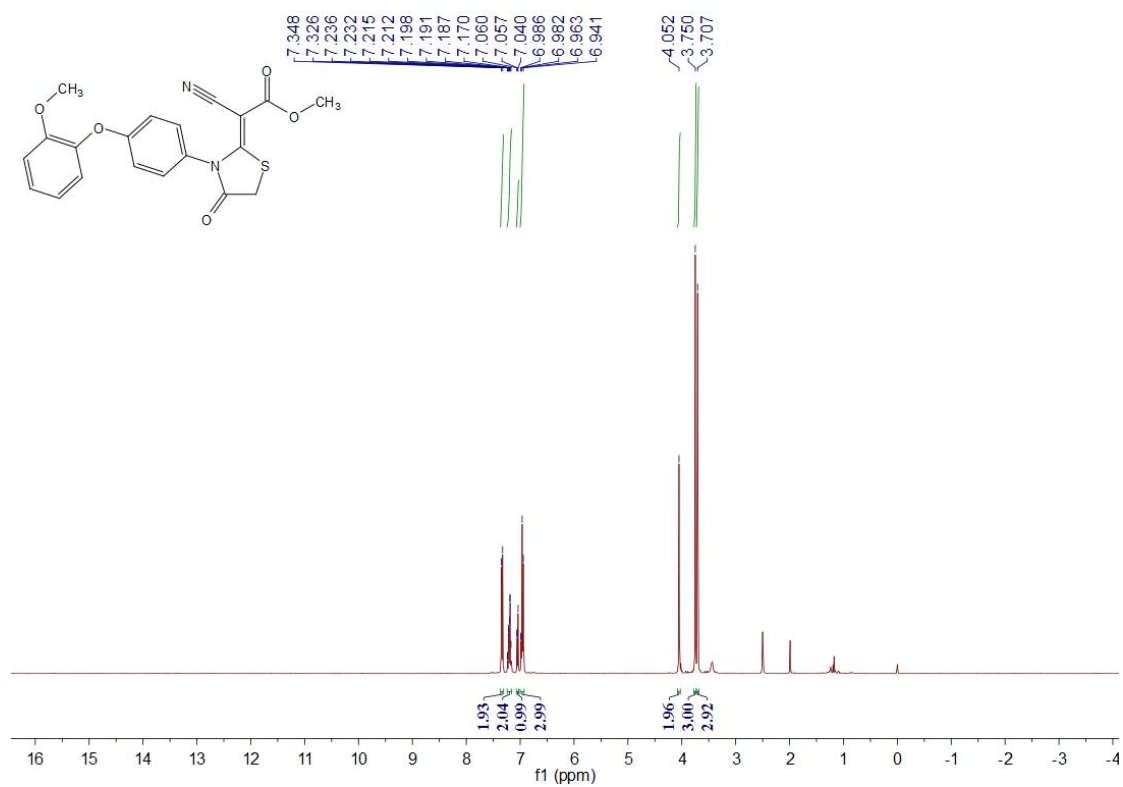
FigureS30.¹⁹F-NMR of compound 18.



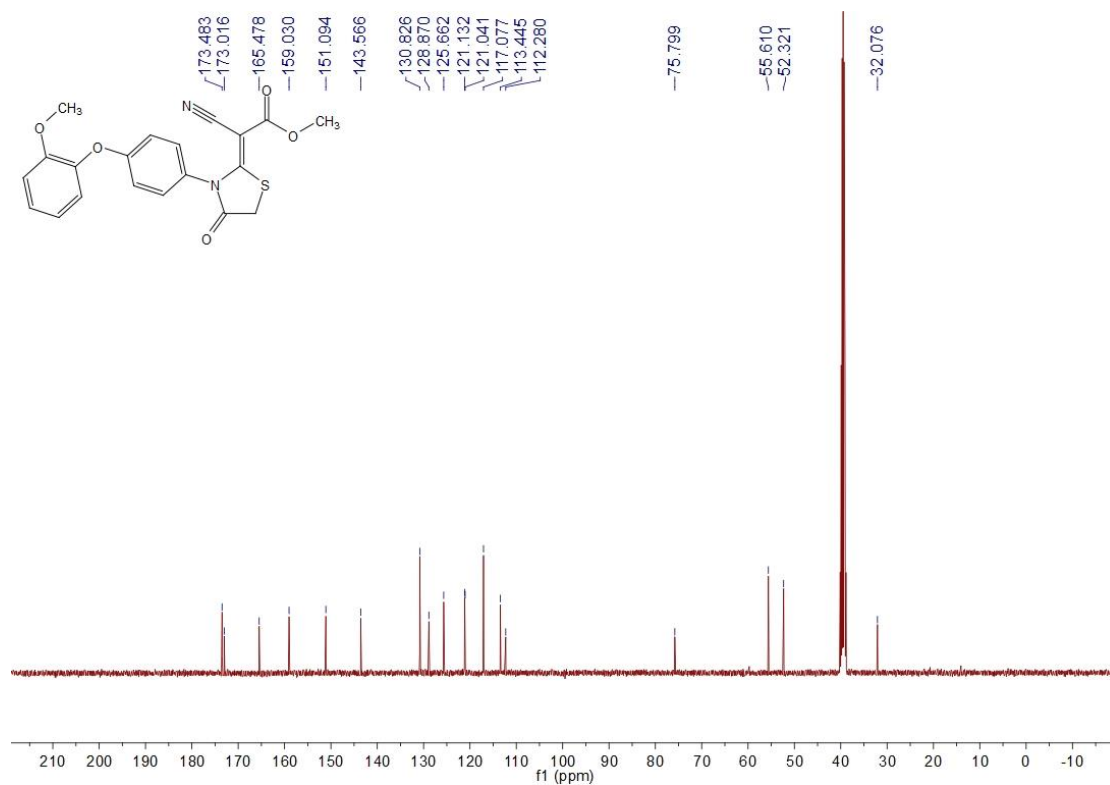
FigureS31.¹H-NMR of compound 19.



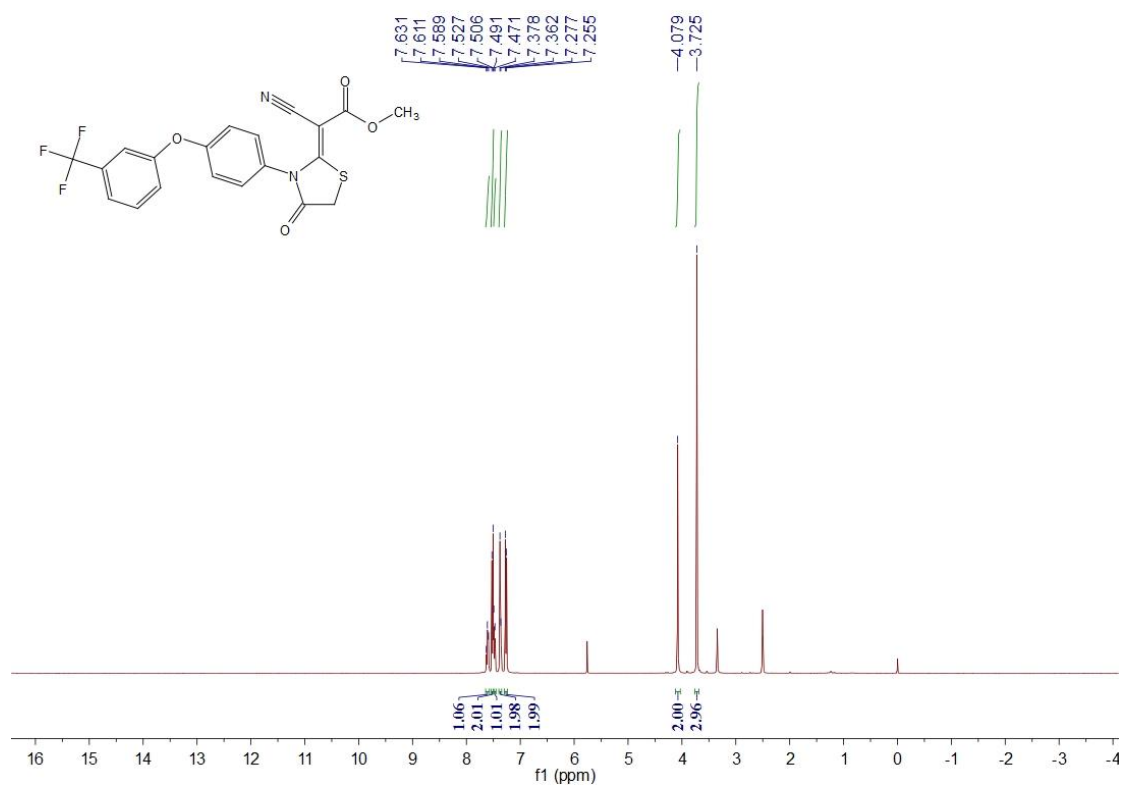
FigureS32.¹³C-NMR of compound 19.



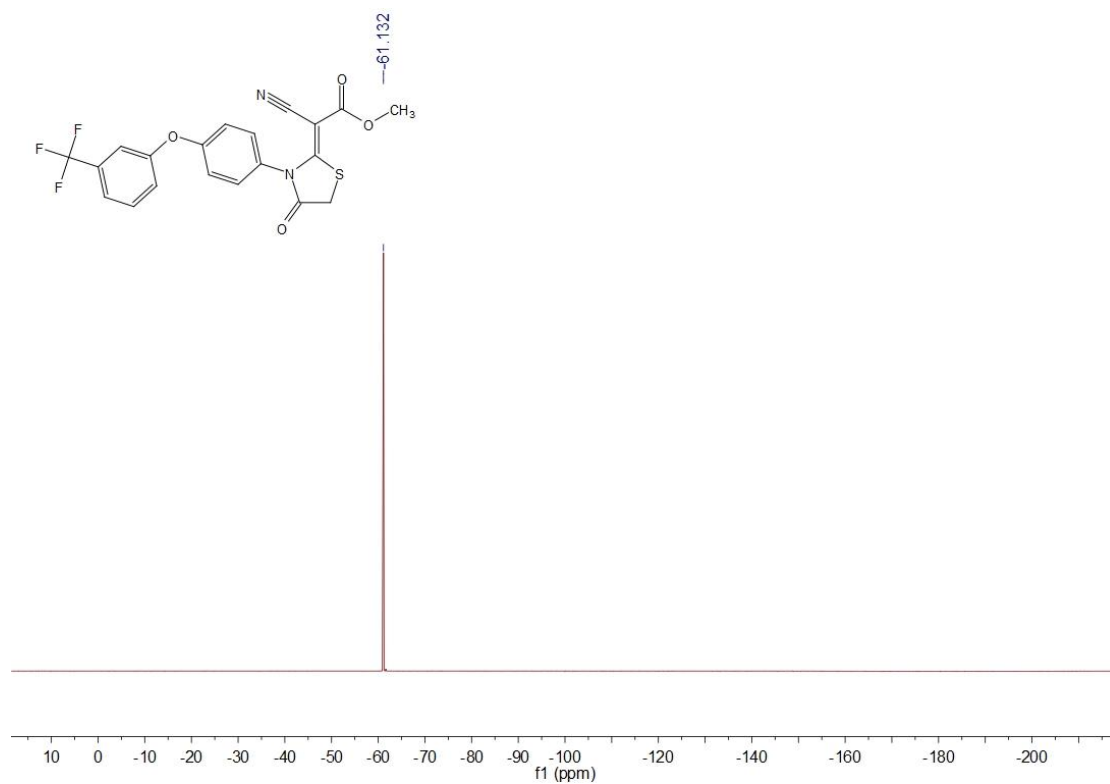
FigureS33. ¹H-NMR of compound 20.



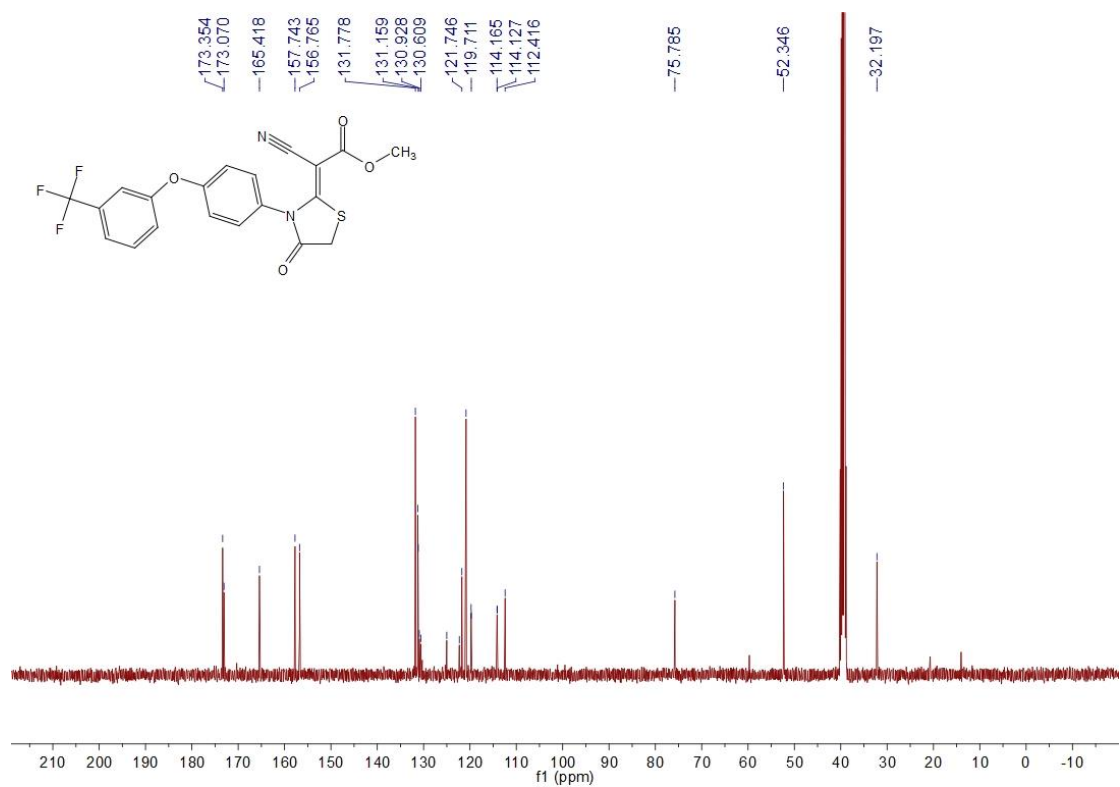
FigureS34. ¹³C-NMR of compound 20.



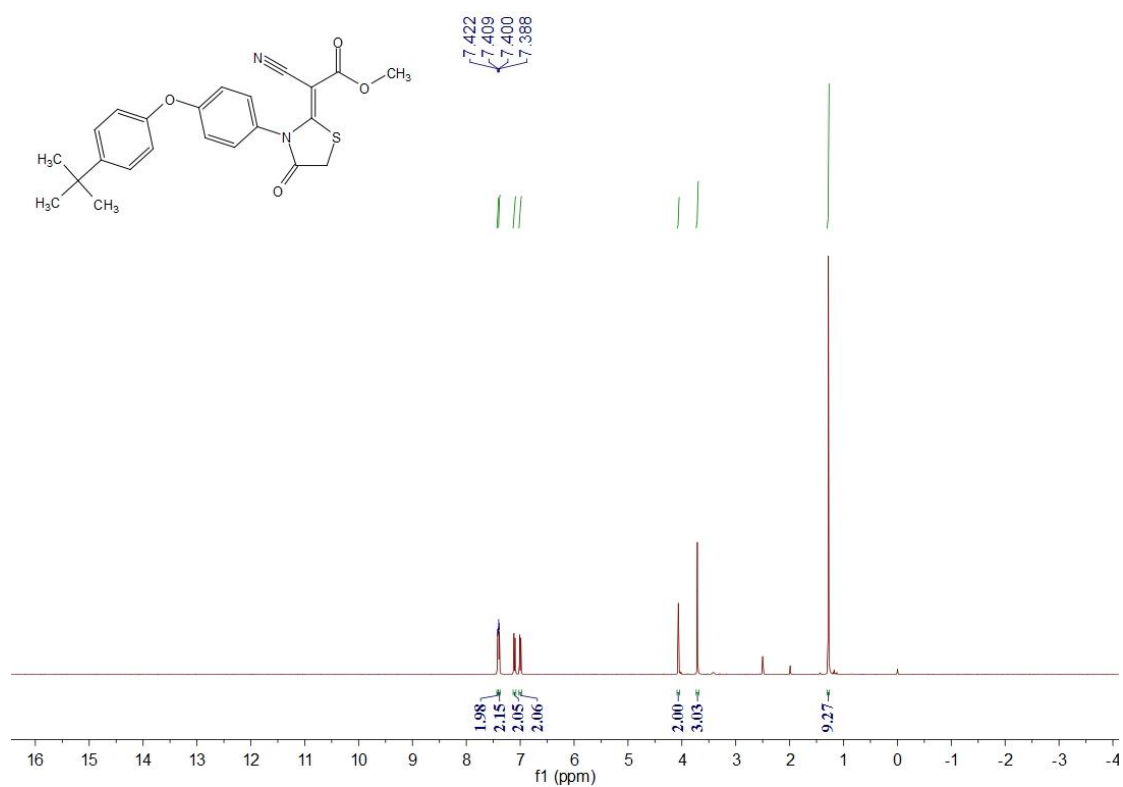
FigureS35. ¹H-NMR of compound 21.



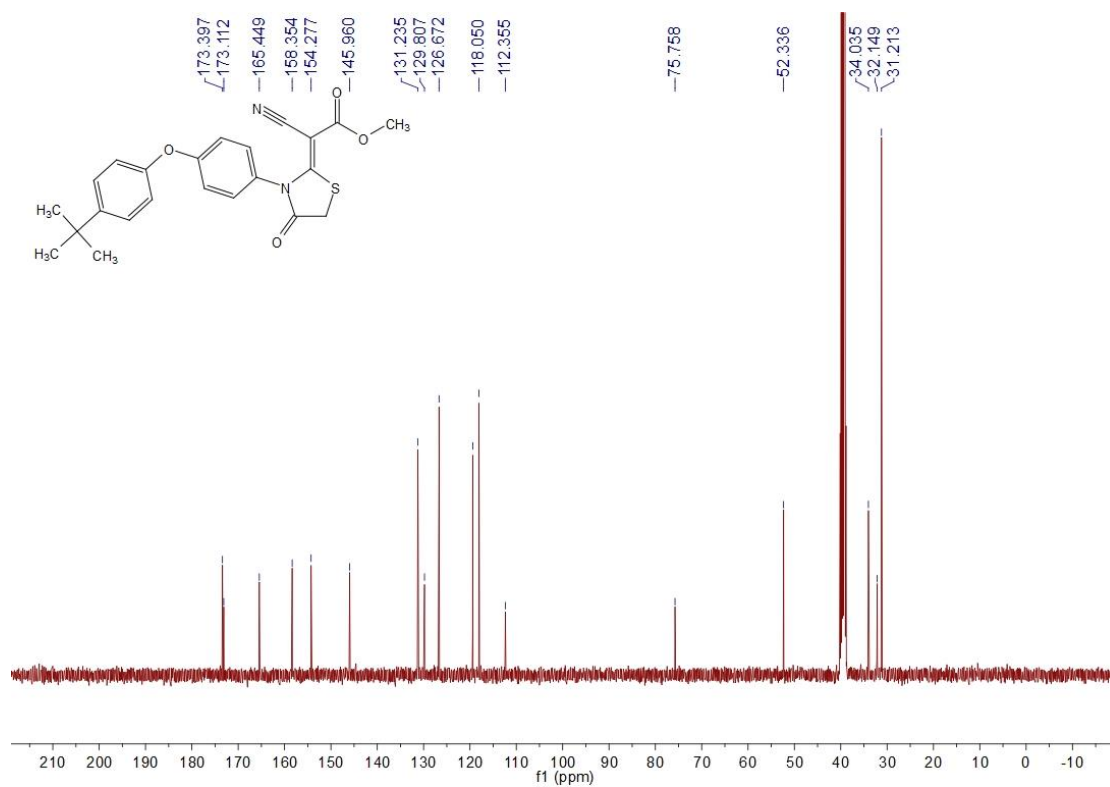
FigureS36. ¹⁹F-NMR of compound 21.



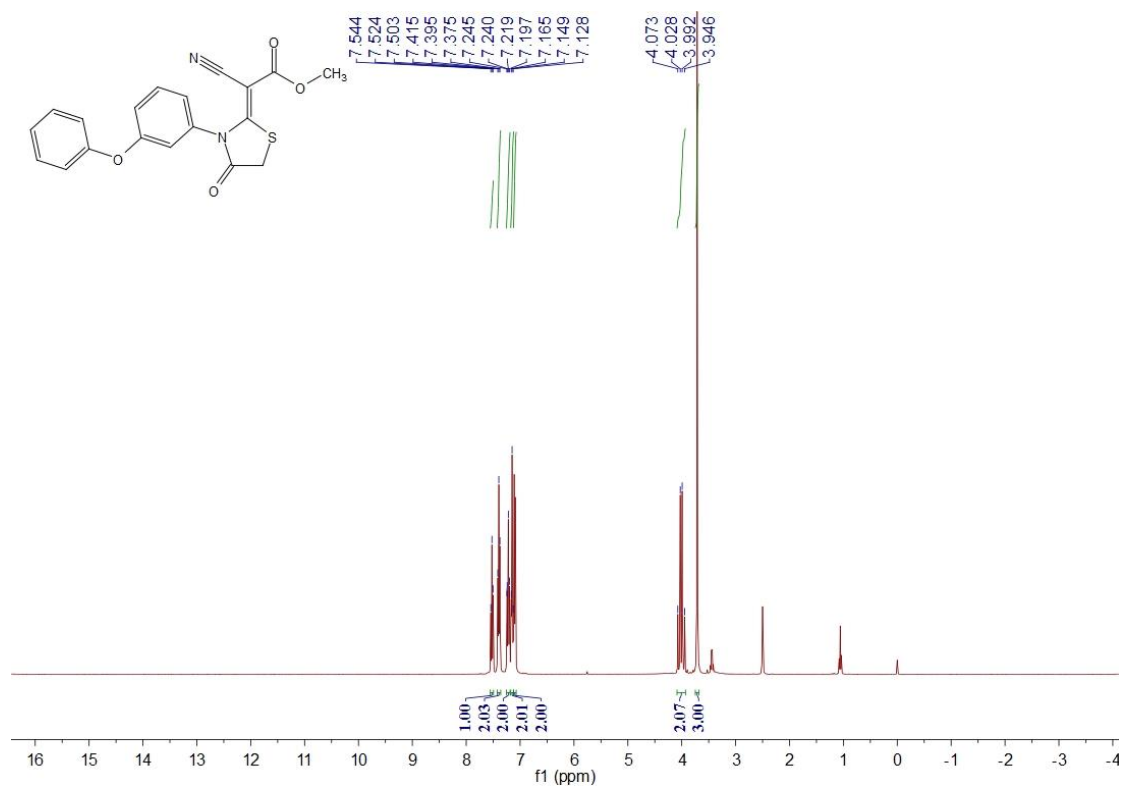
FigureS37.¹³C-NMR of compound 21.



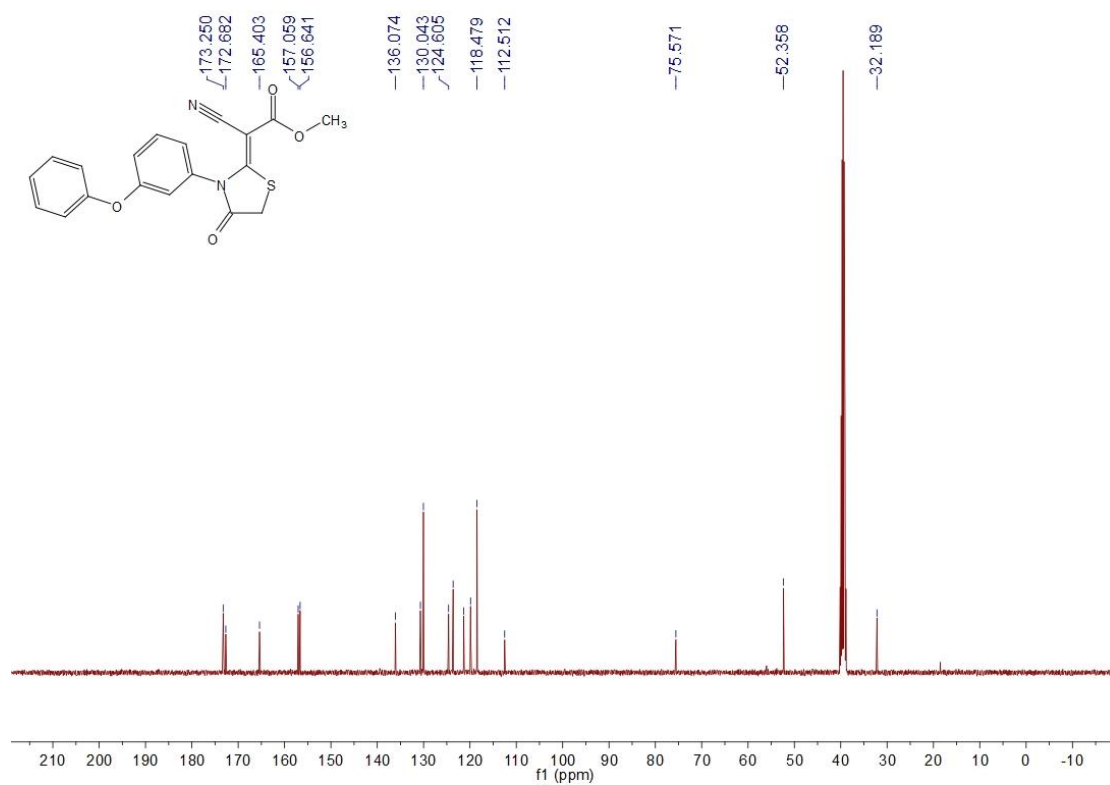
FigureS38.¹H-NMR of compound 22.



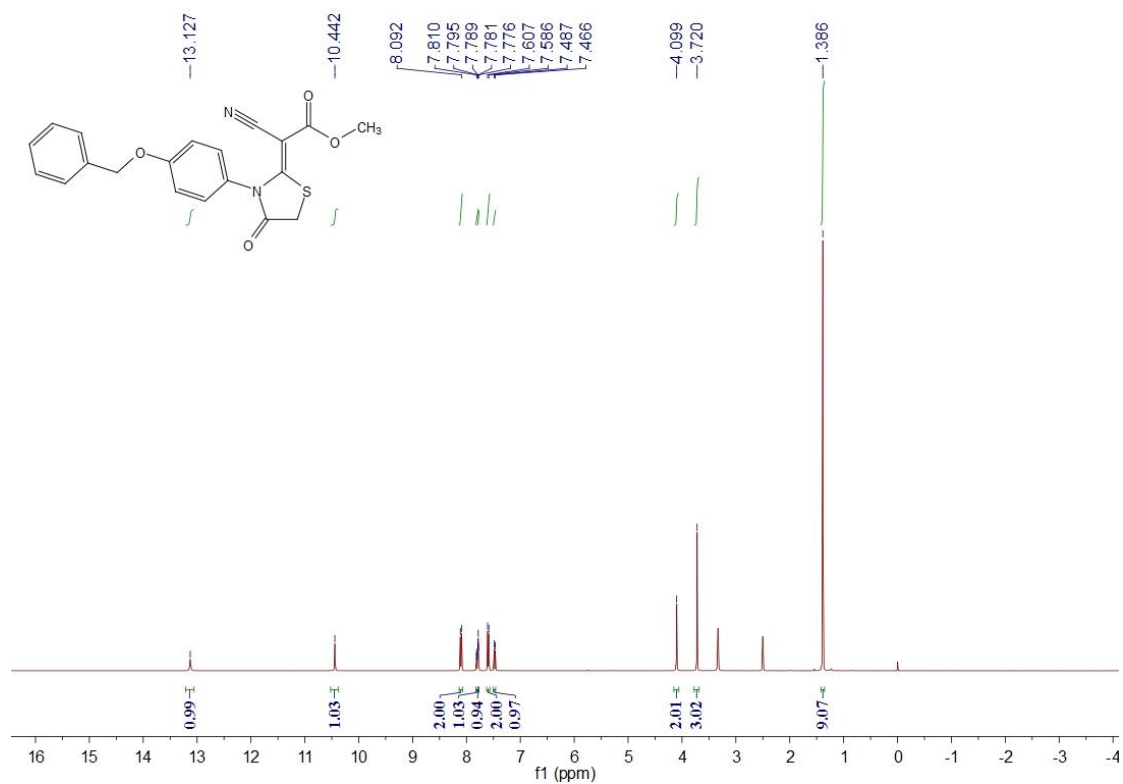
FigureS39.¹³C-NMR of compound 22.



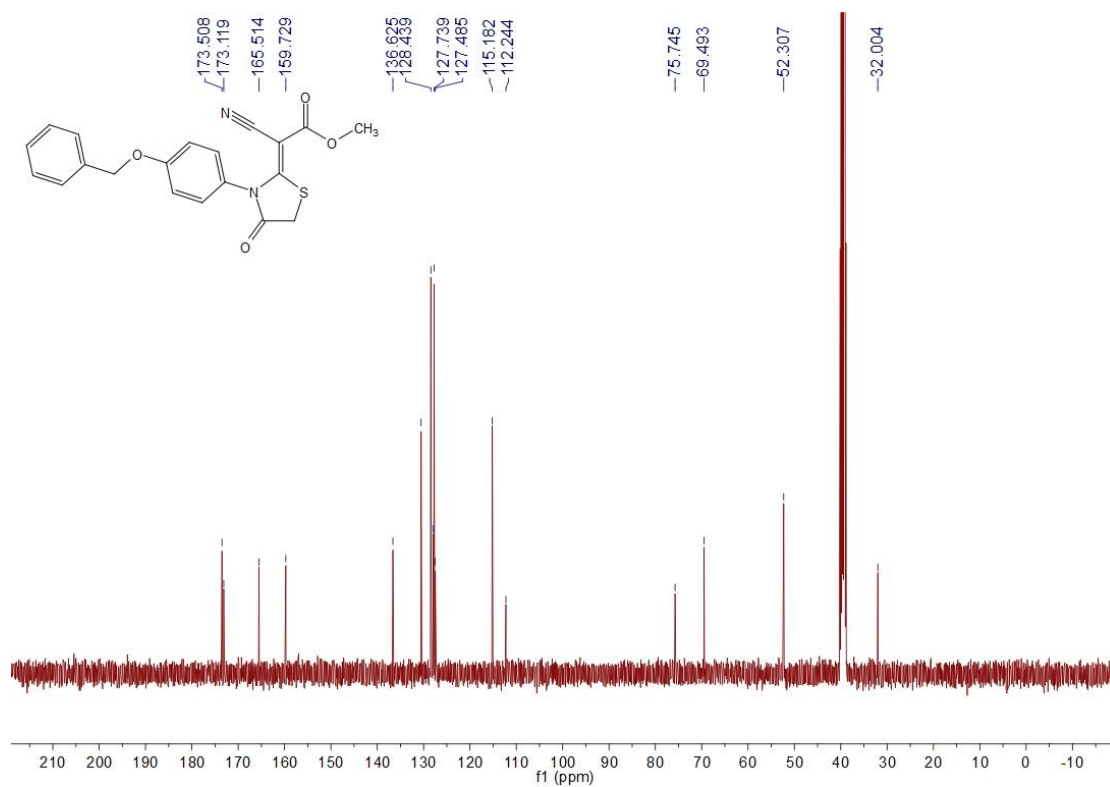
FigureS40.¹H-NMR of compound 23.



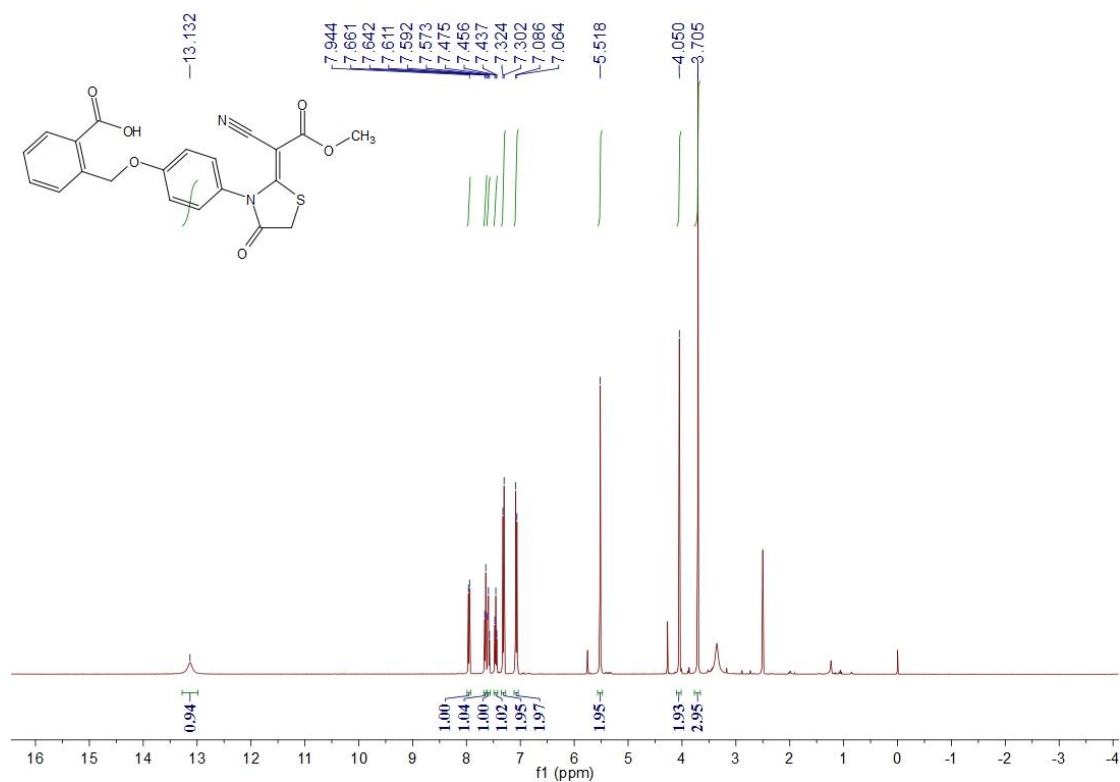
FigureS41. ¹³C-NMR of compound 23.



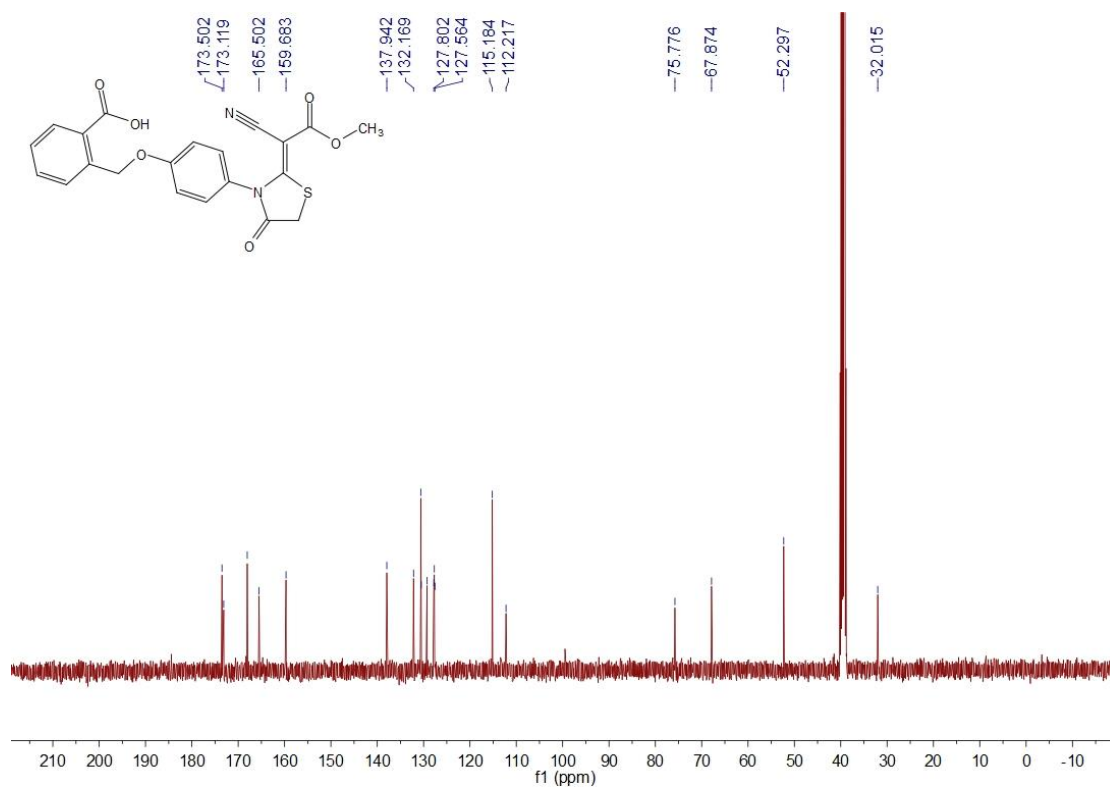
FigureS42. ¹H-NMR of compound 24.



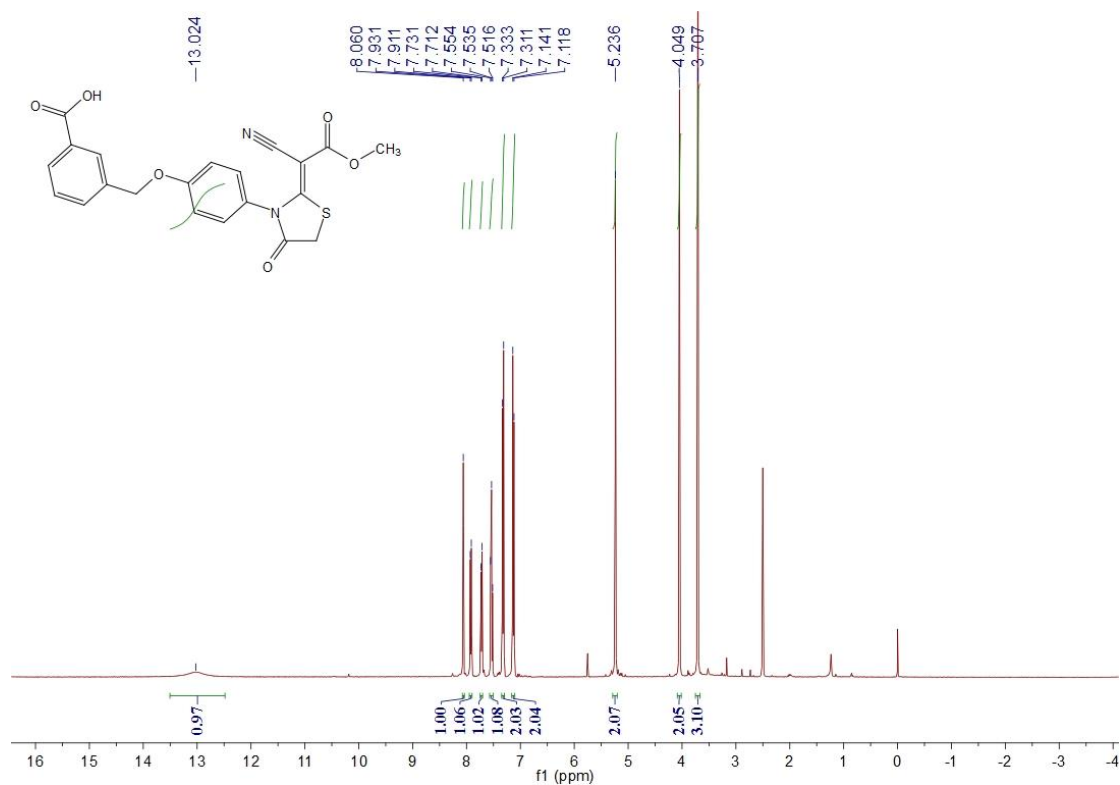
FigureS43. ¹³C-NMR of compound 24.



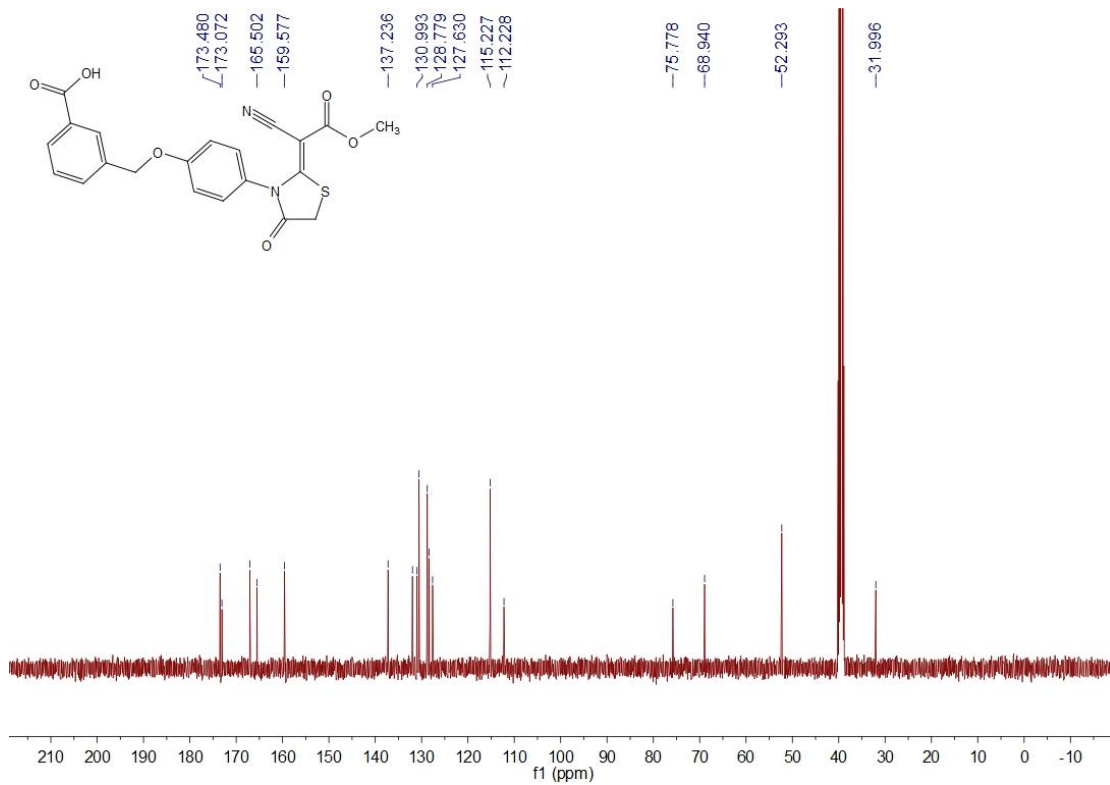
FigureS44. ¹H-NMR of compound 25.



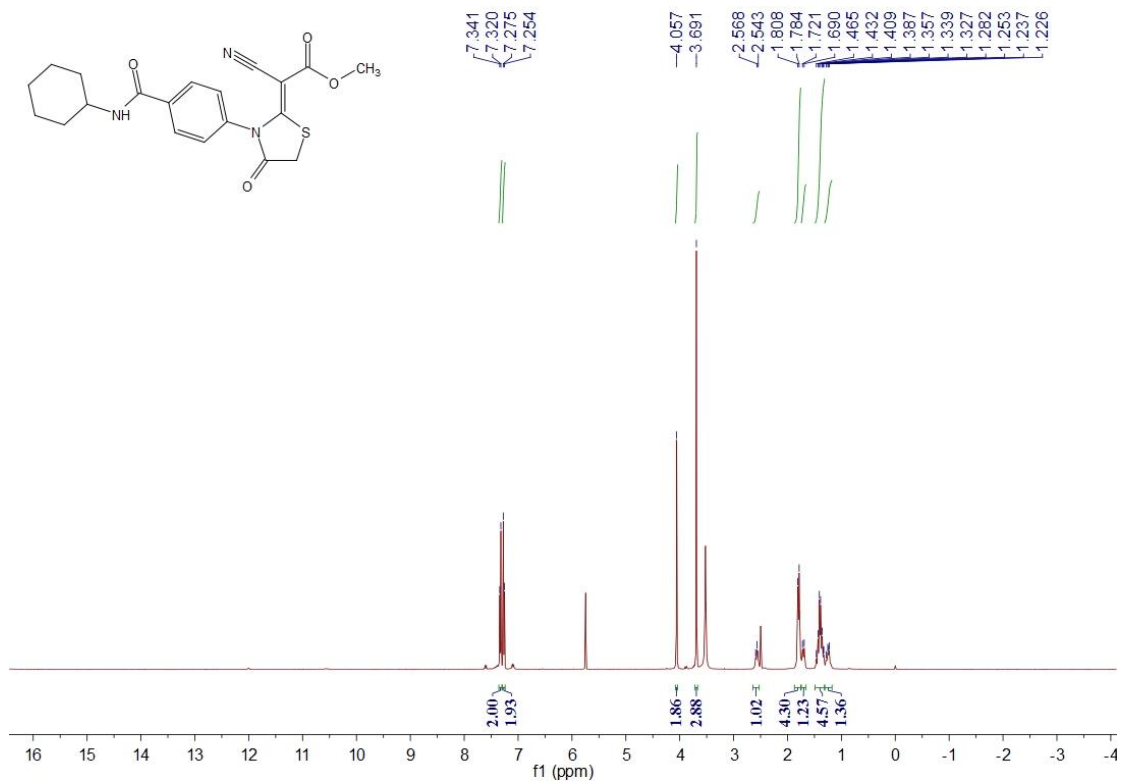
FigureS45. ¹³C-NMR of compound 25.



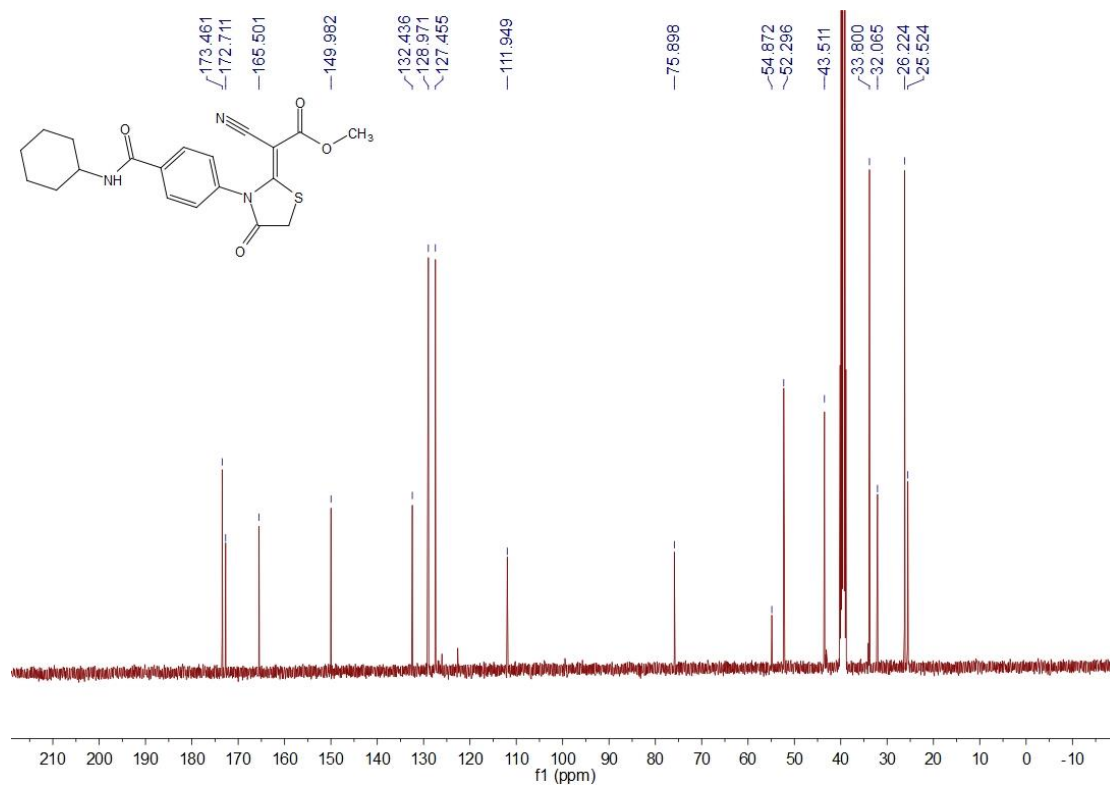
FigureS46. ¹H-NMR of compound 26.



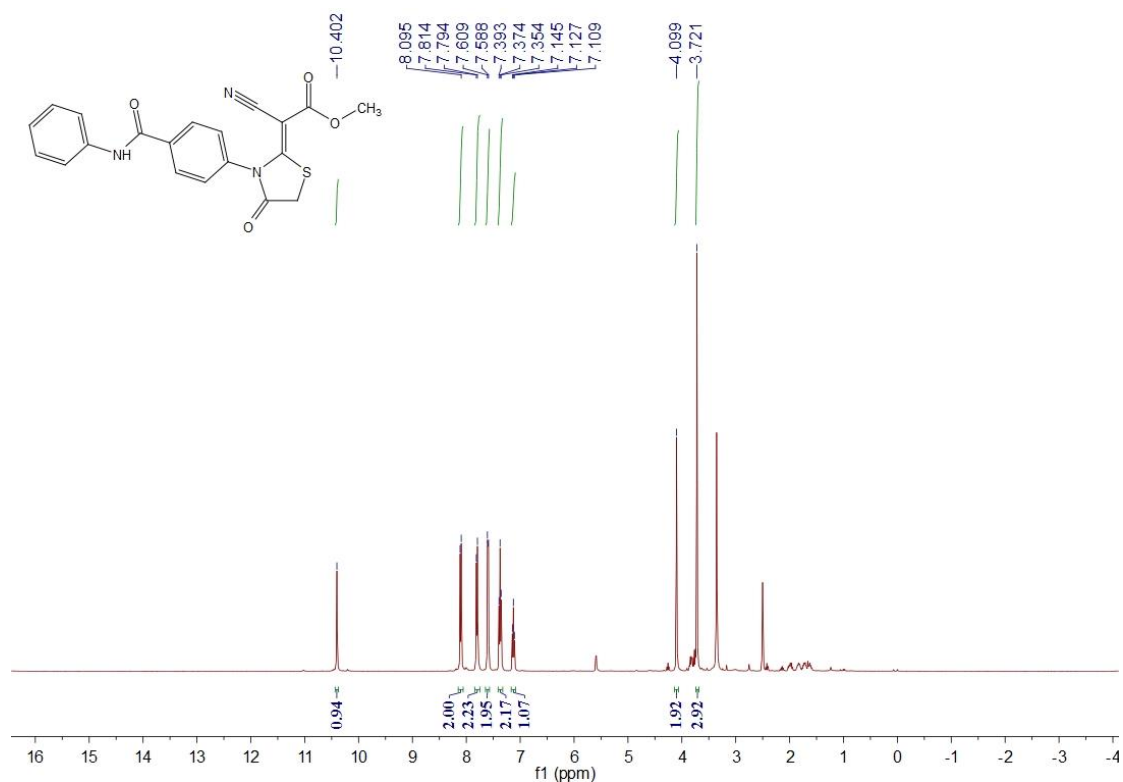
FigureS47.¹³C-NMR of compound **26**.



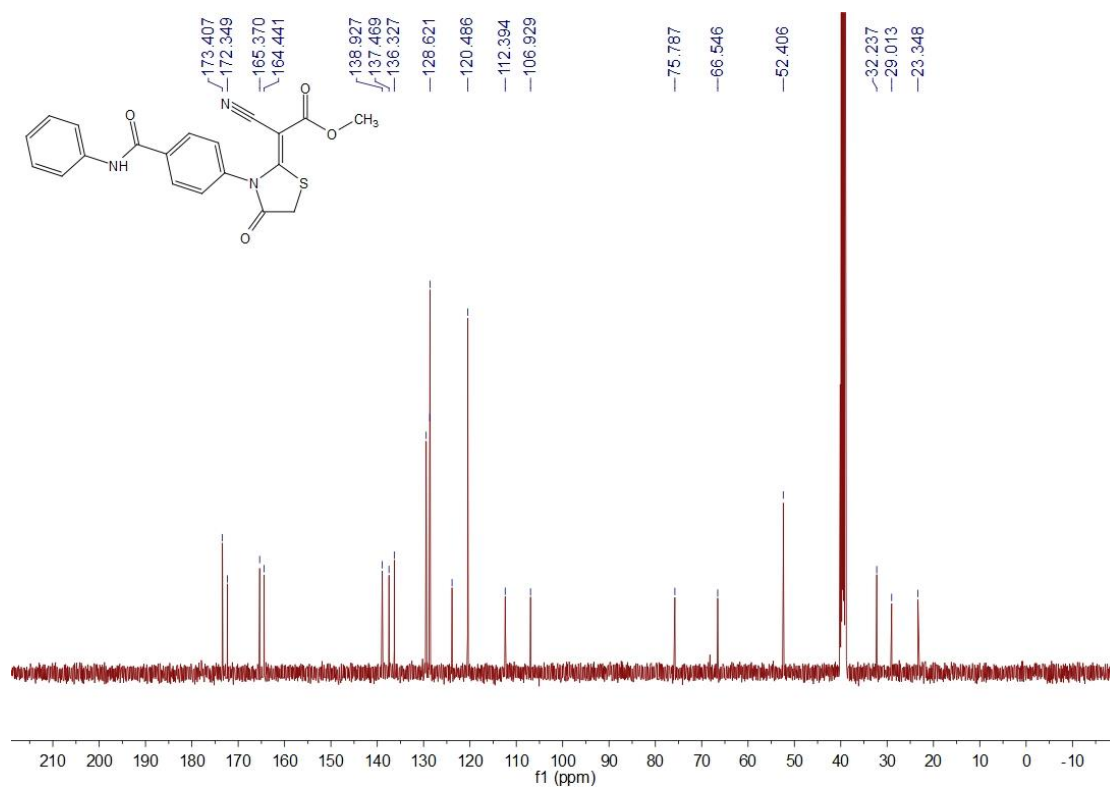
FigureS48.¹H-NMR of compound **27**.



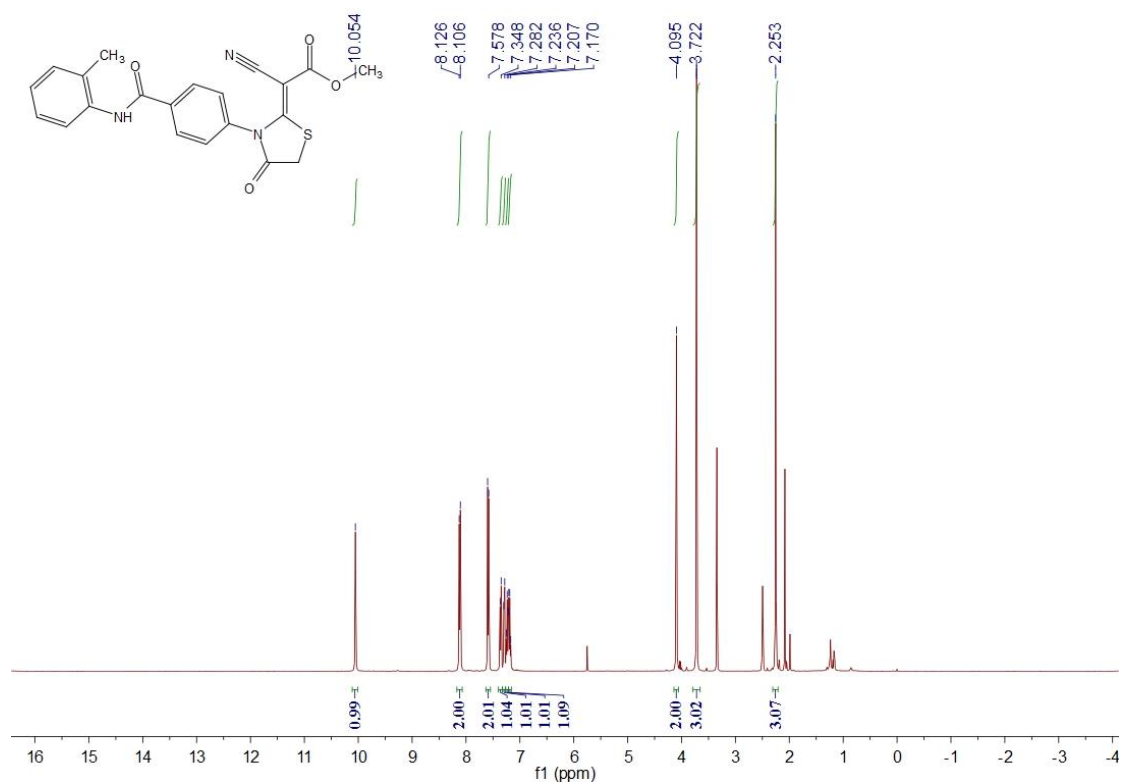
FigureS49. ¹³C-NMR of compound 27.



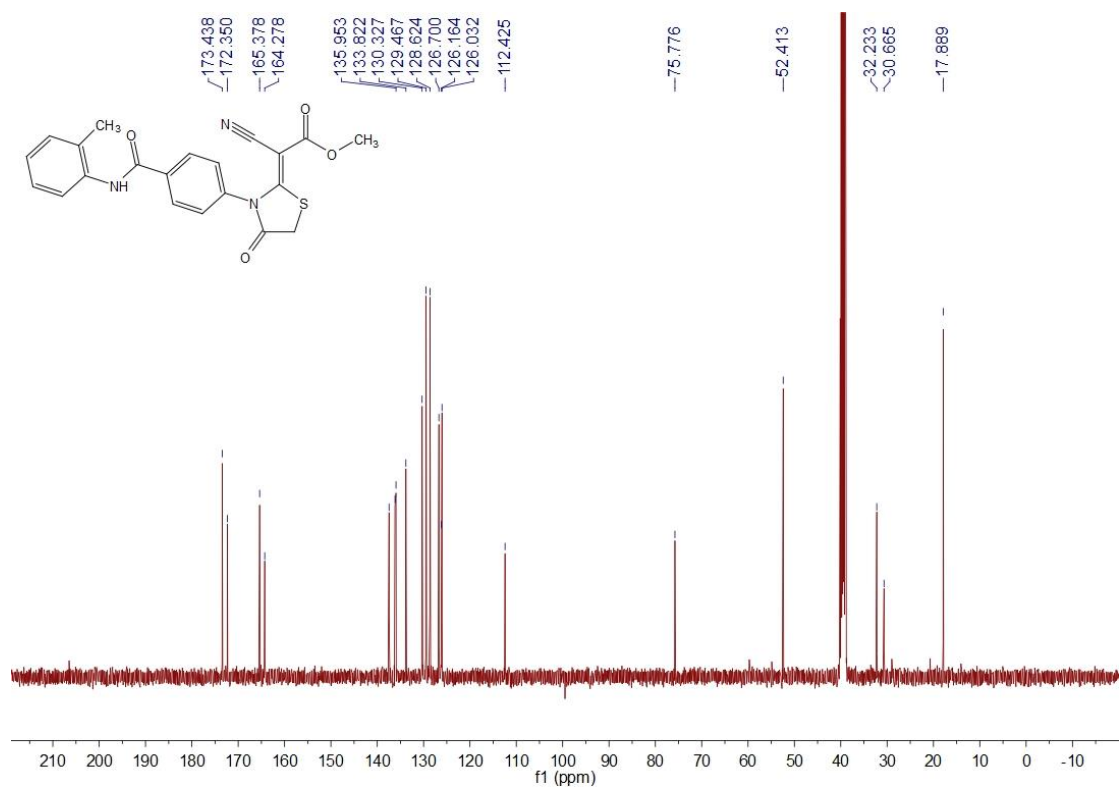
FigureS50. ¹H-NMR of compound 28.



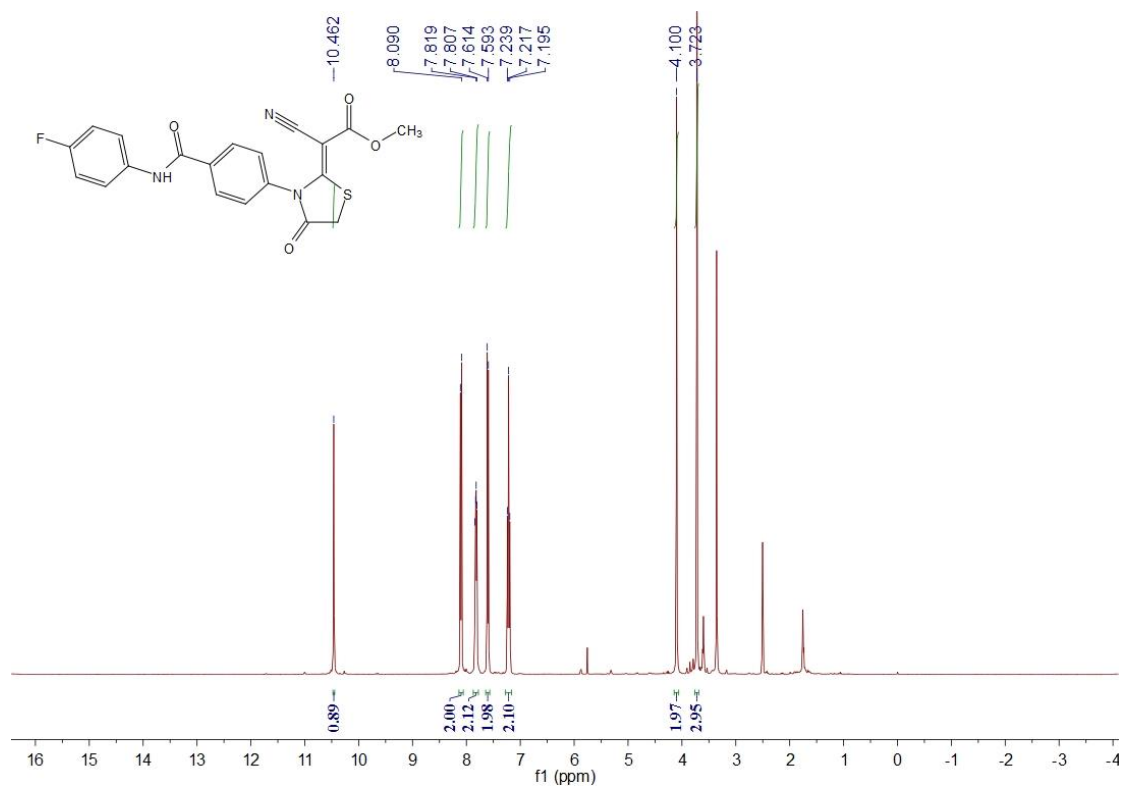
FigureS51. ¹³C-NMR of compound 28.



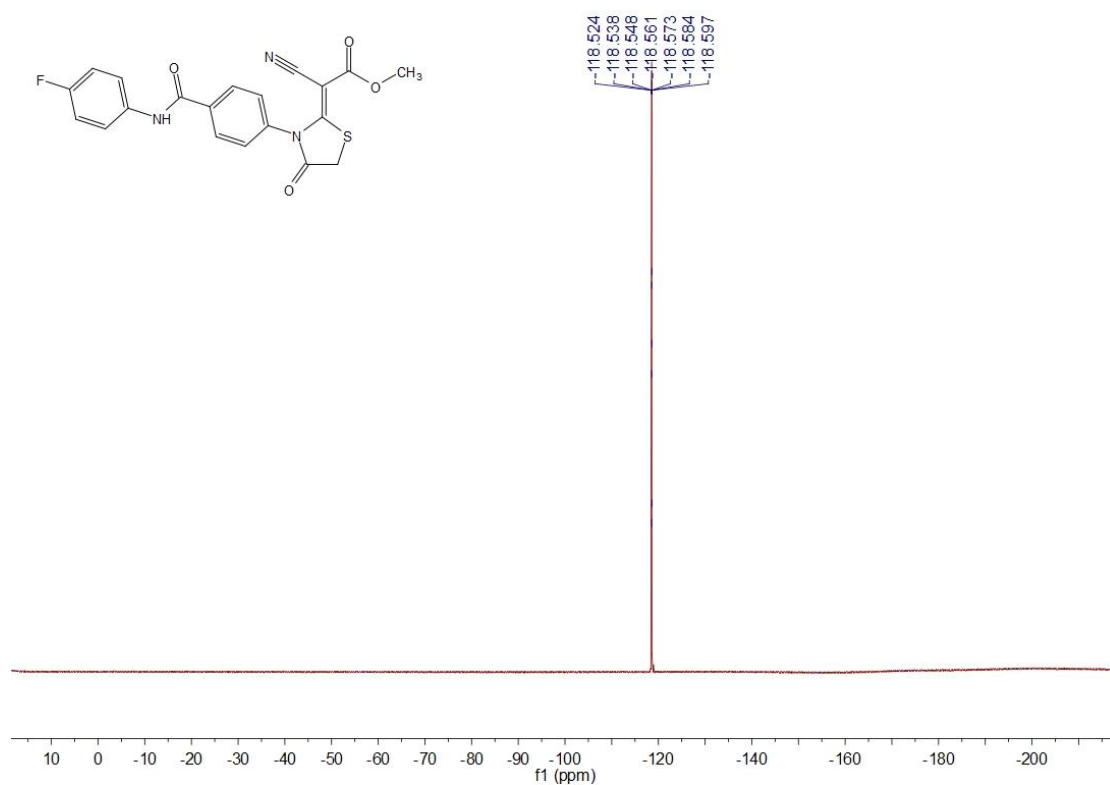
FigureS52. ¹H-NMR of compound 29.



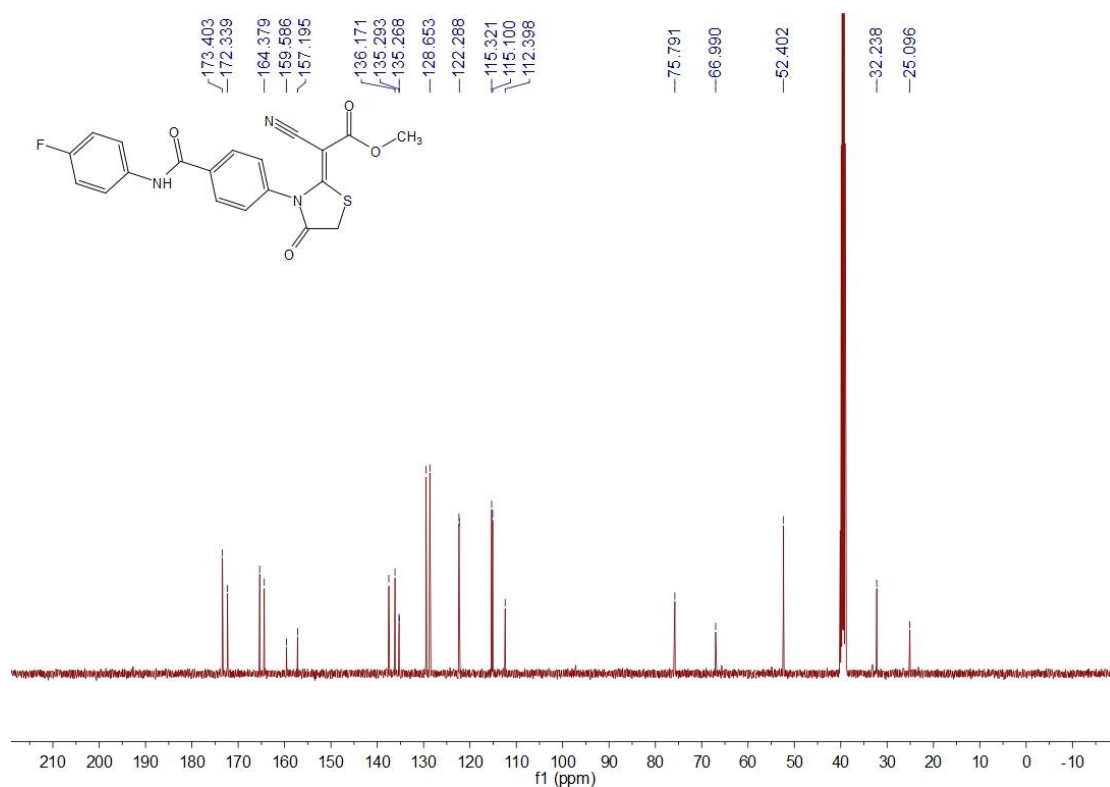
FigureS53. ¹³C-NMR of compound 29.



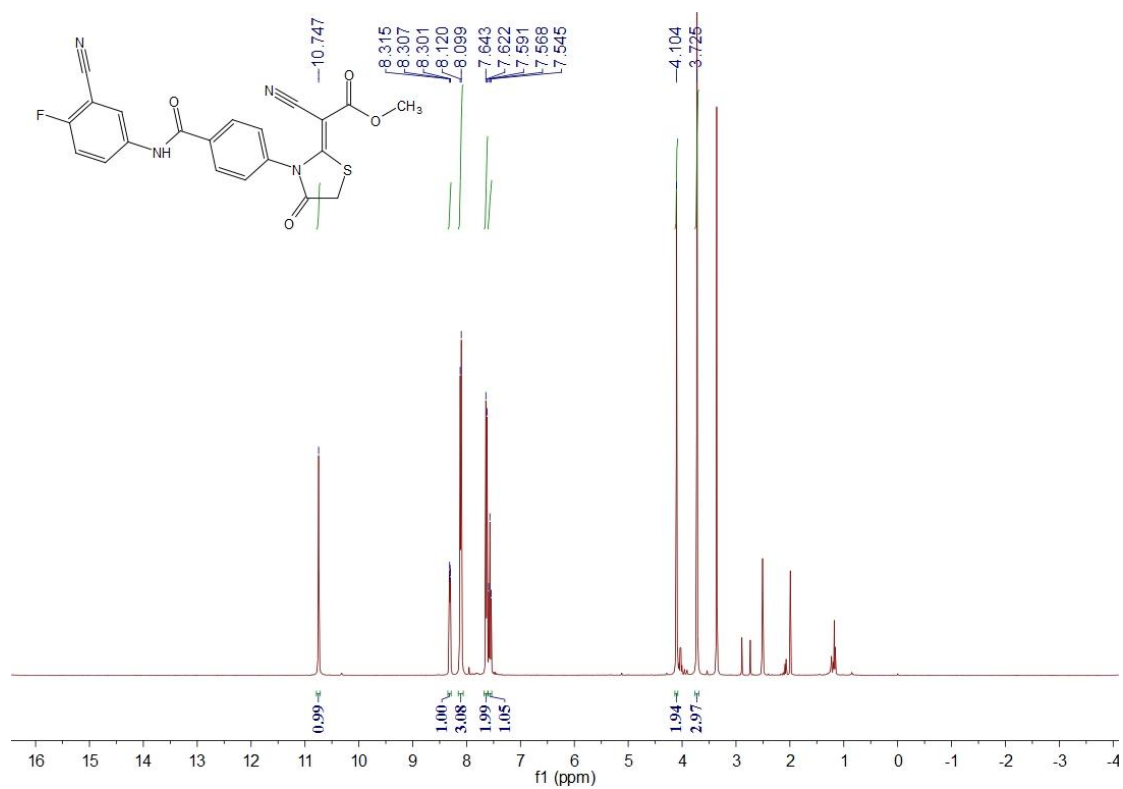
FigureS54. ¹H-NMR of compound 30.



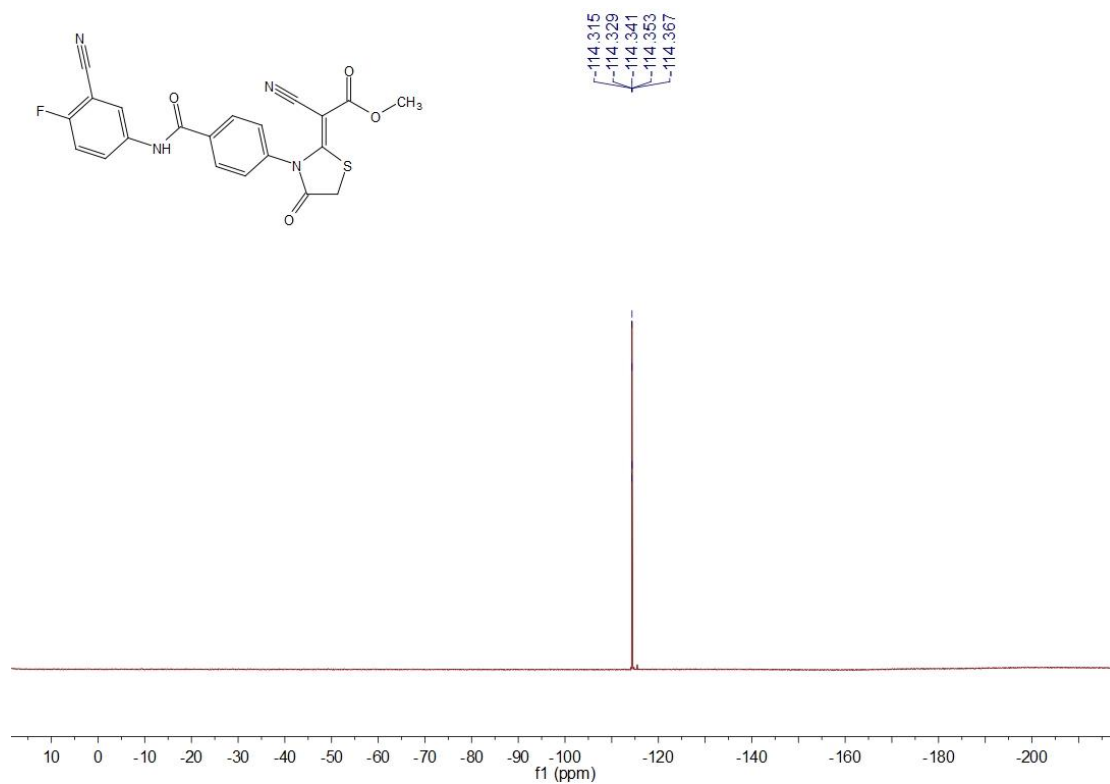
FigureS55. ¹⁹F-NMR of compound 30.



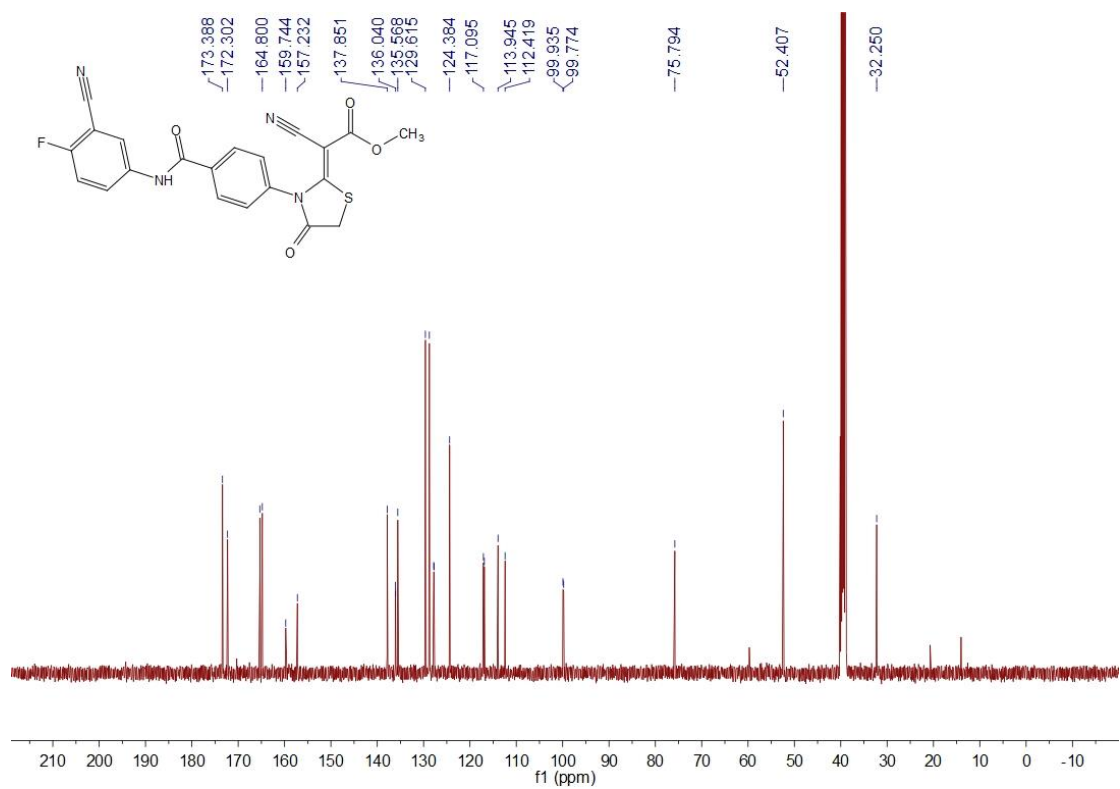
FigureS56. ¹³C-NMR of compound 30.



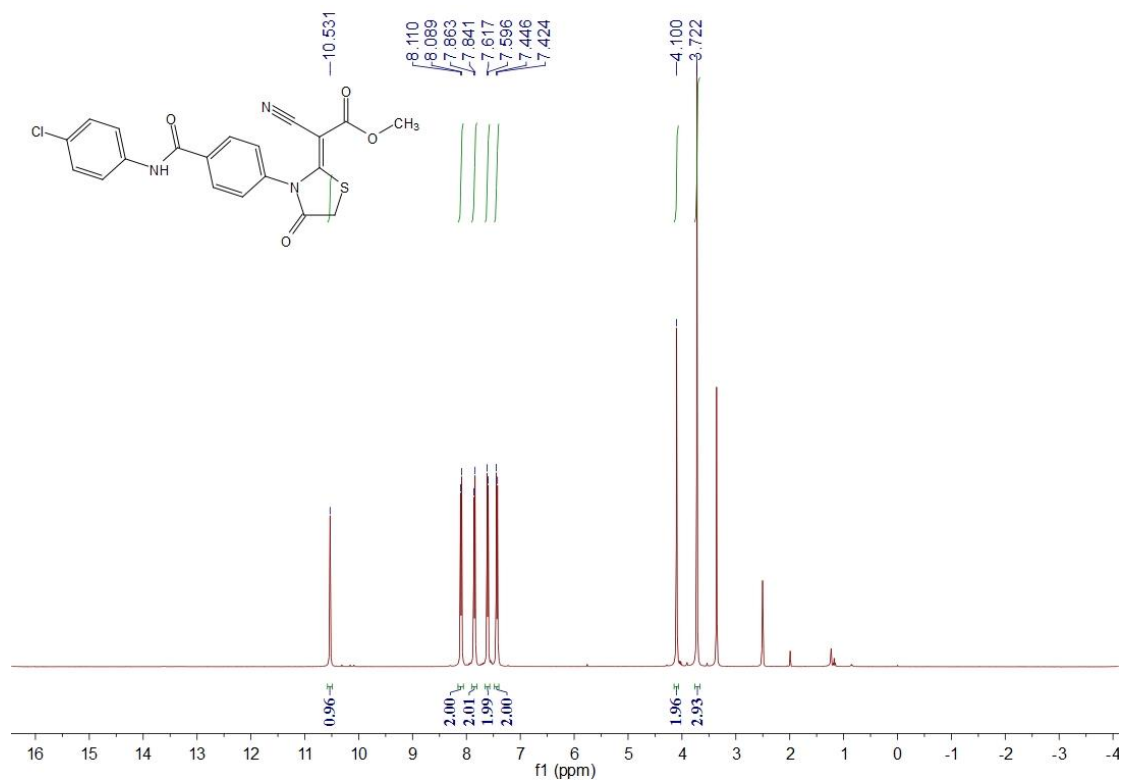
FigureS57. ¹H-NMR of compound 31.



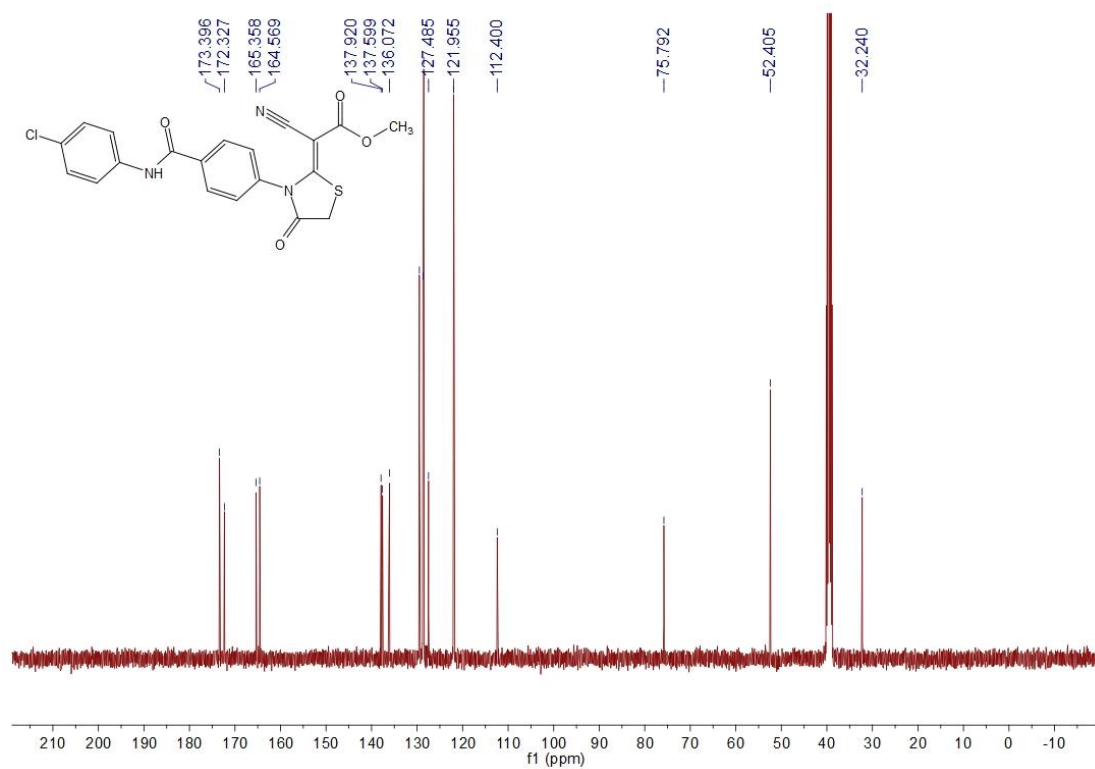
FigureS58. ¹⁹F-NMR of compound 31.



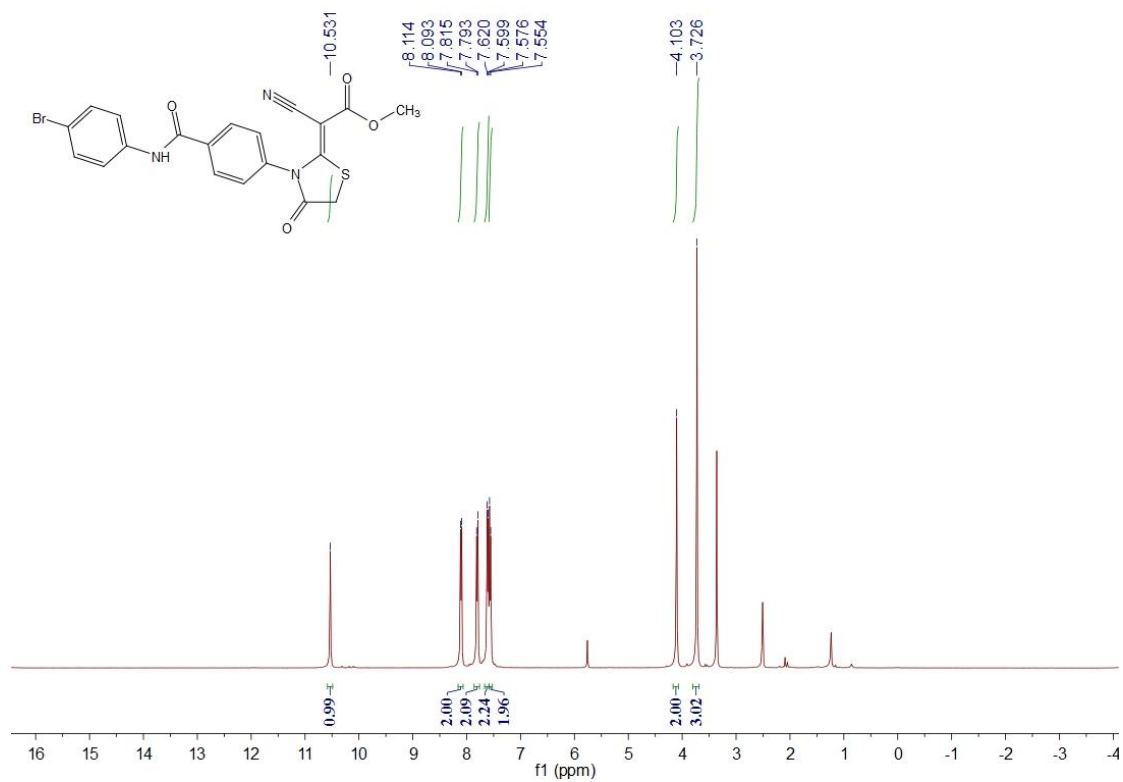
FigureS59.¹³C-NMR of compound 31.



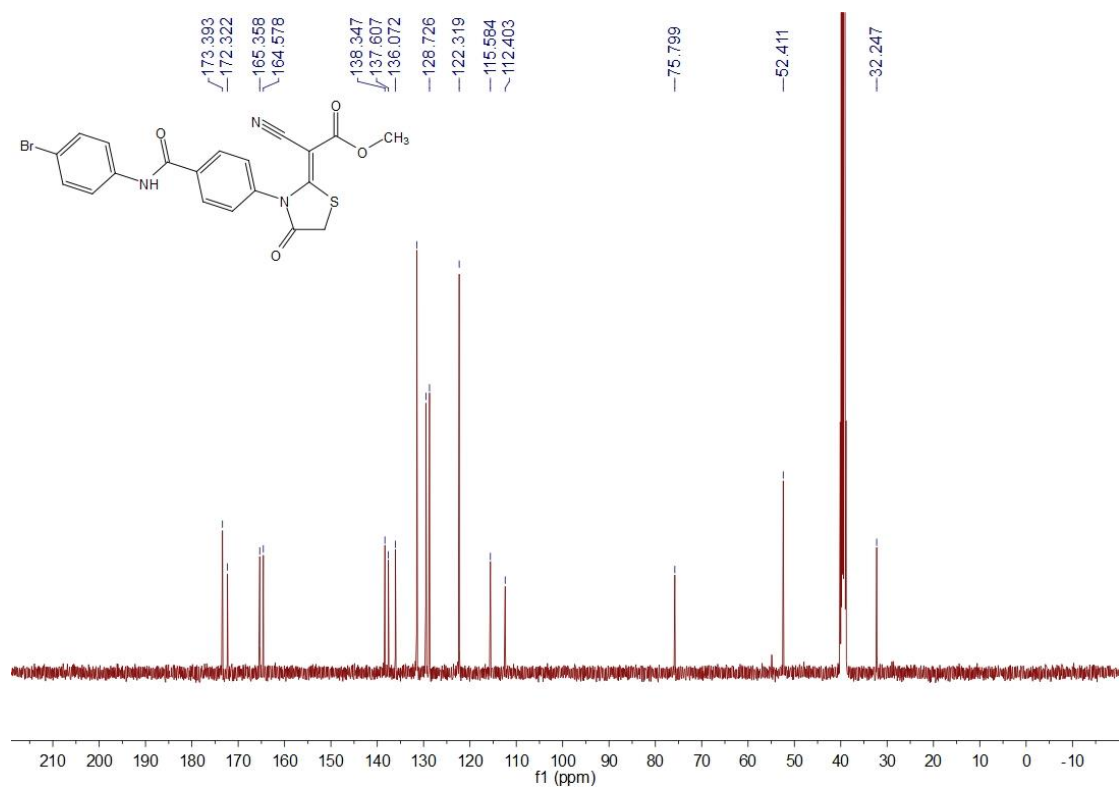
FigureS60.¹H-NMR of compound 32.



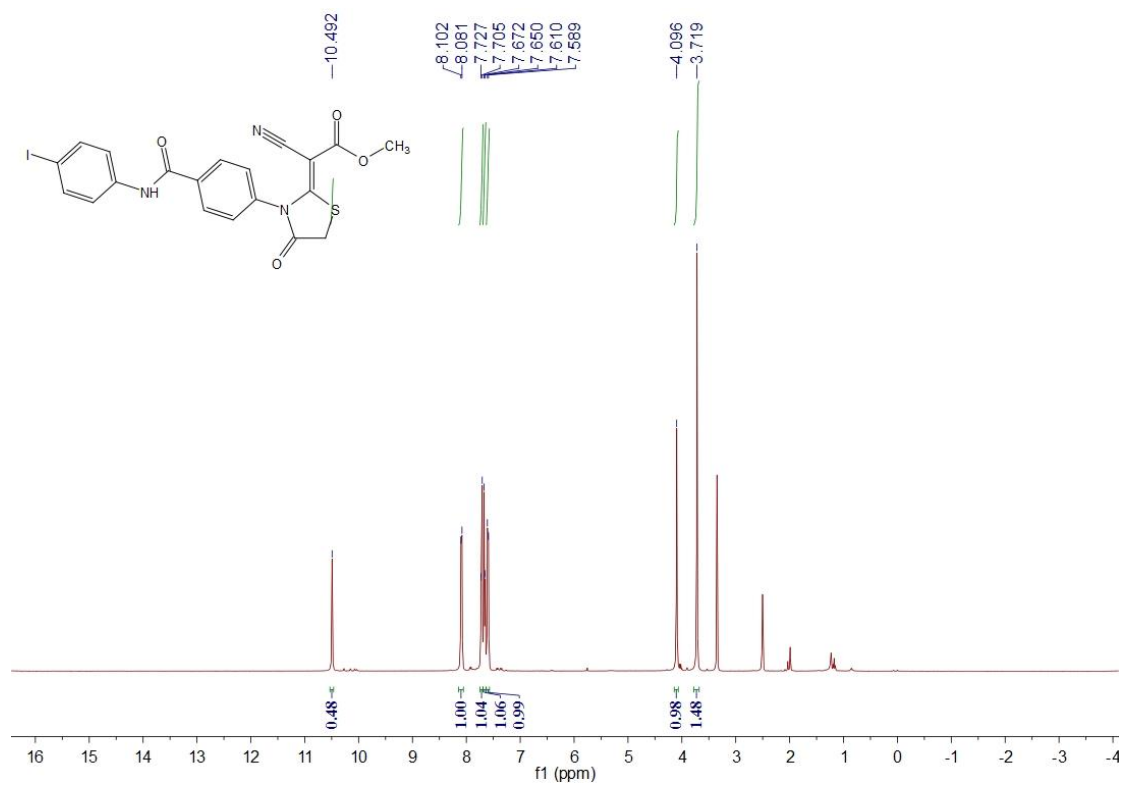
FigureS61. ¹³C-NMR of compound 32.



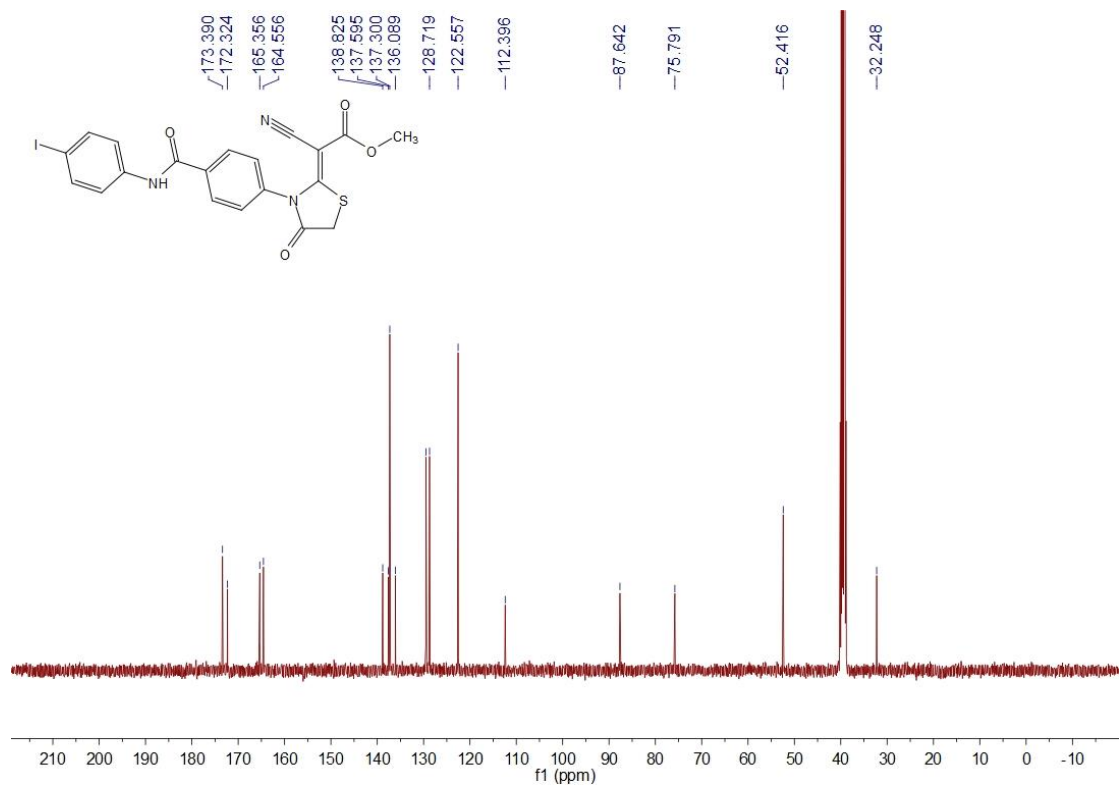
FigureS62. ¹H-NMR of compound 33.



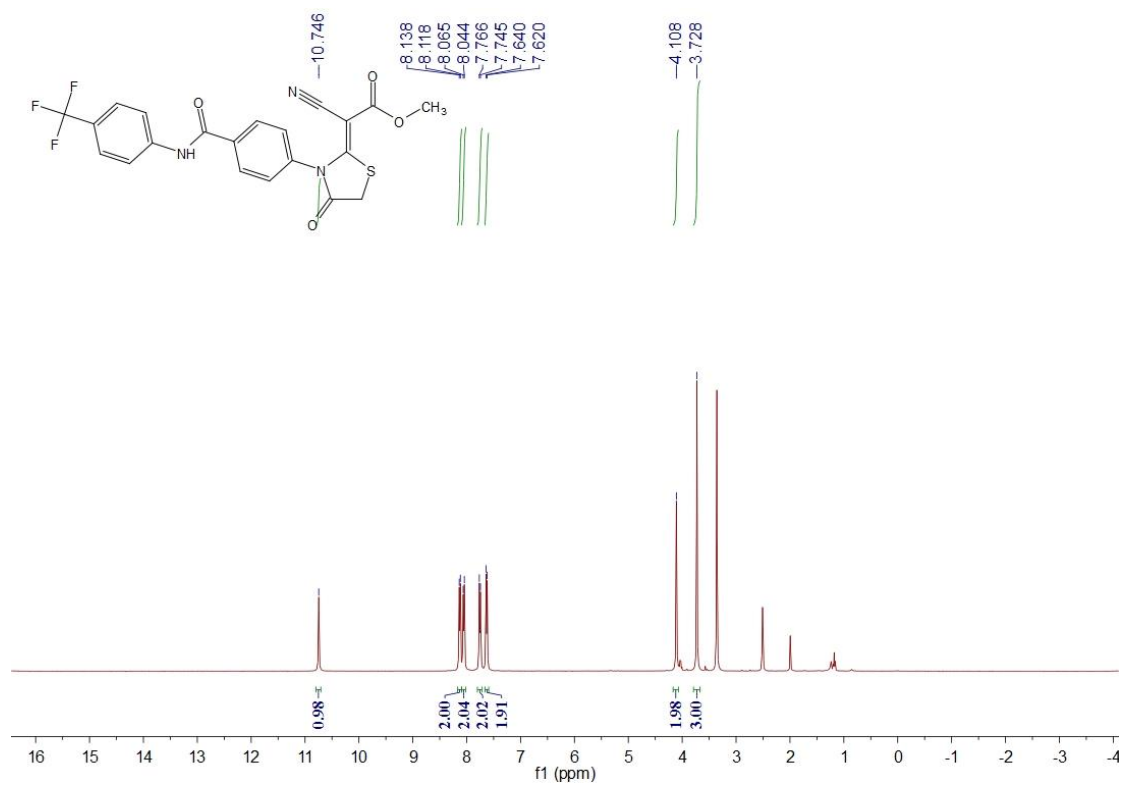
FigureS63. ¹³C-NMR of compound 33.



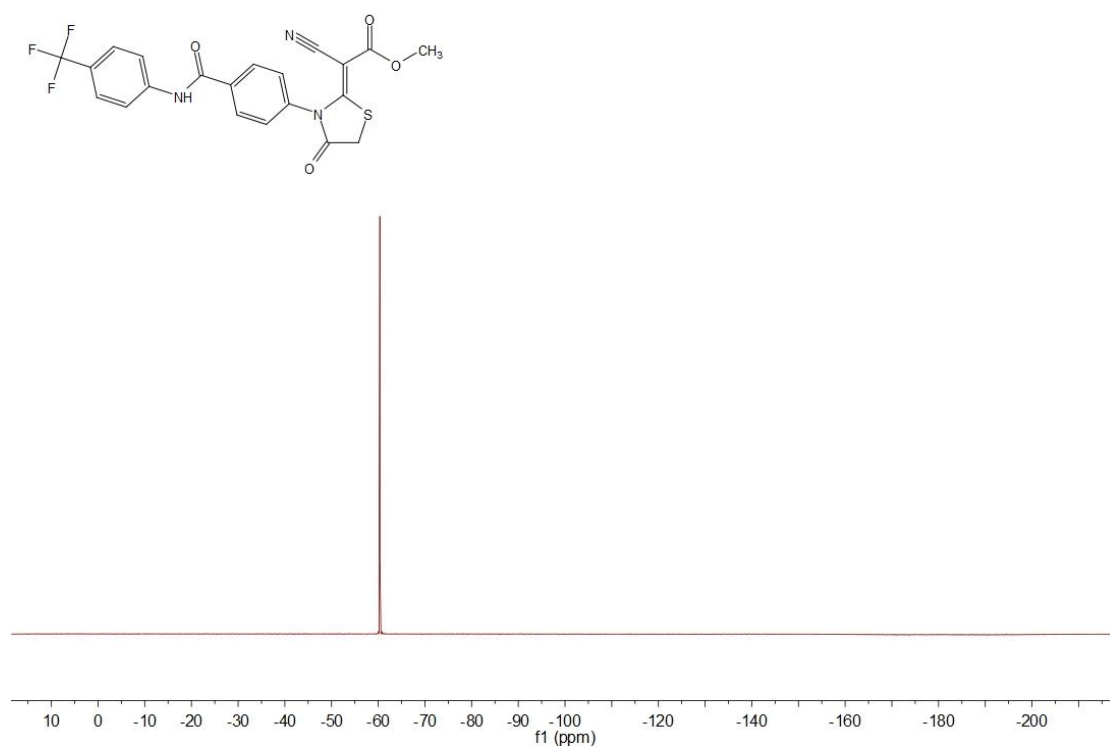
FigureS64. ¹H-NMR of compound 34.



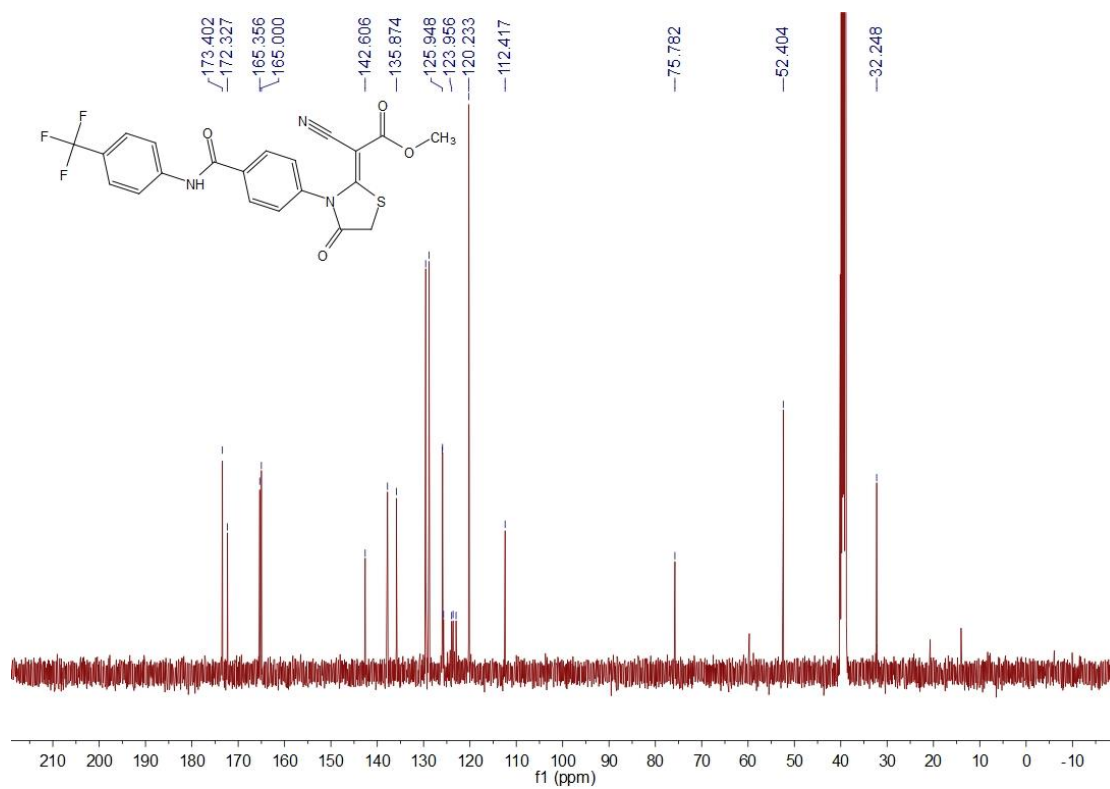
FigureS65. ¹³C-NMR of compound 34.



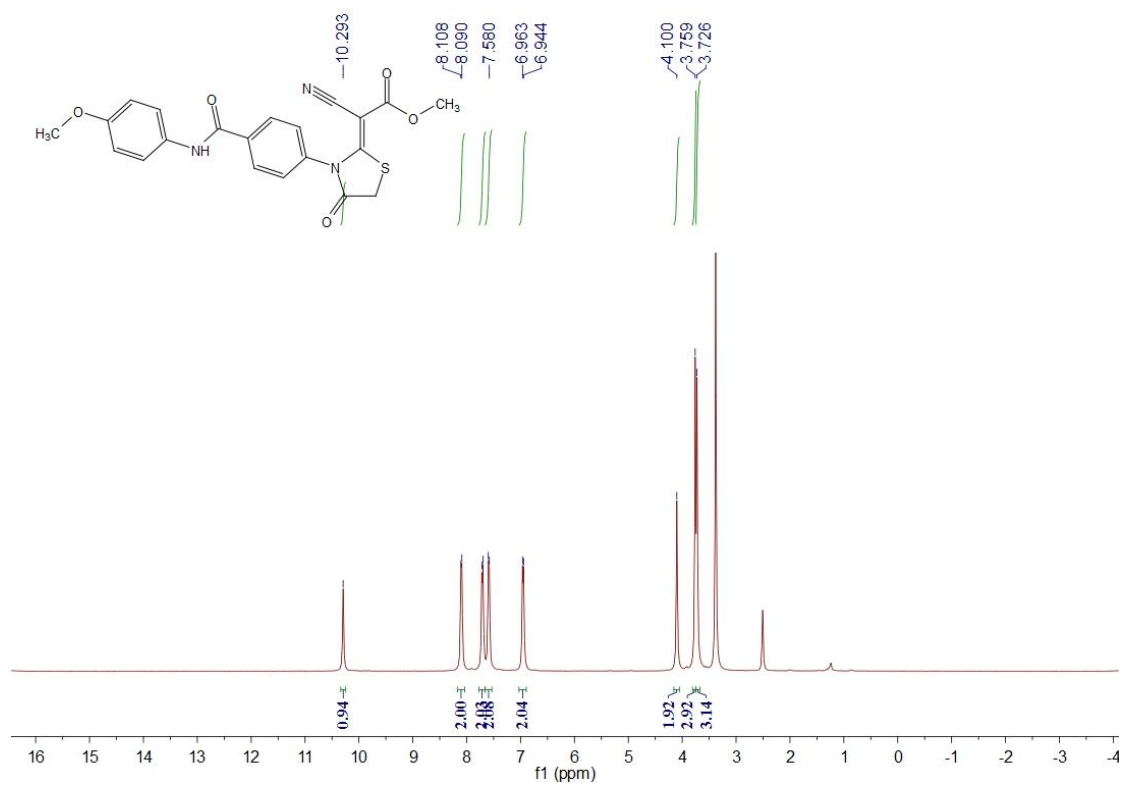
FigureS66. ¹H-NMR of compound 35.



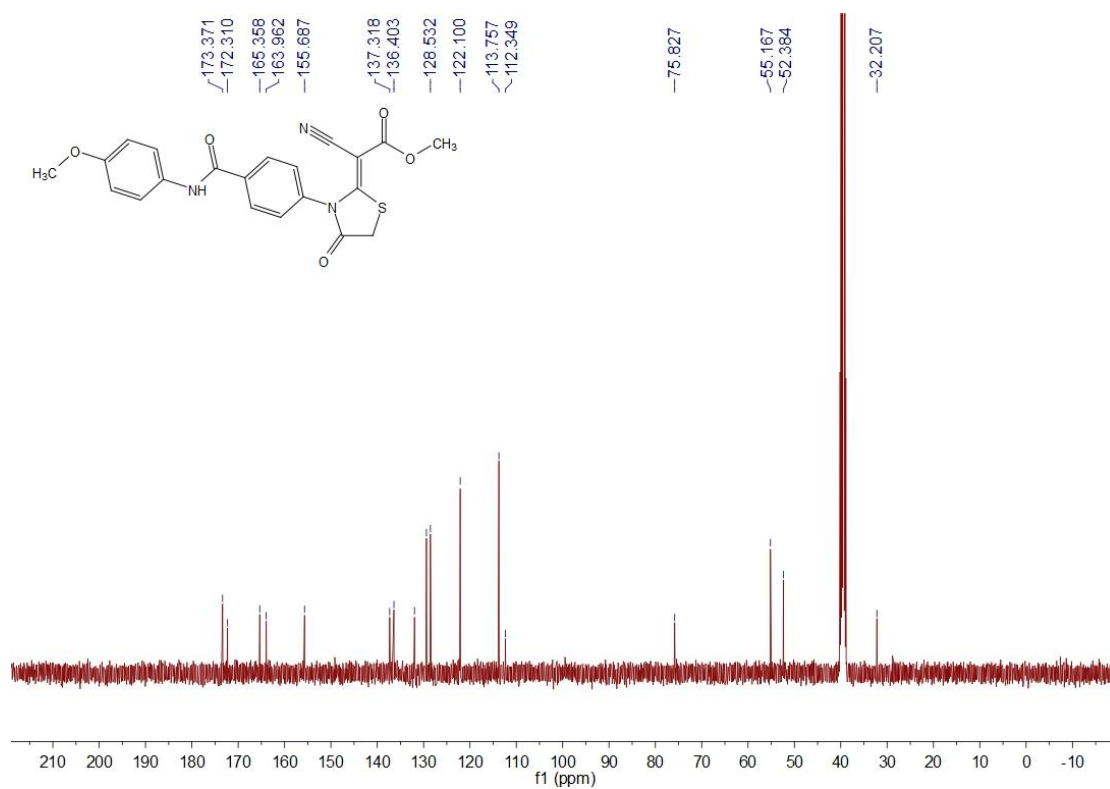
FigureS67. ^{19}F -NMR of compound 35.



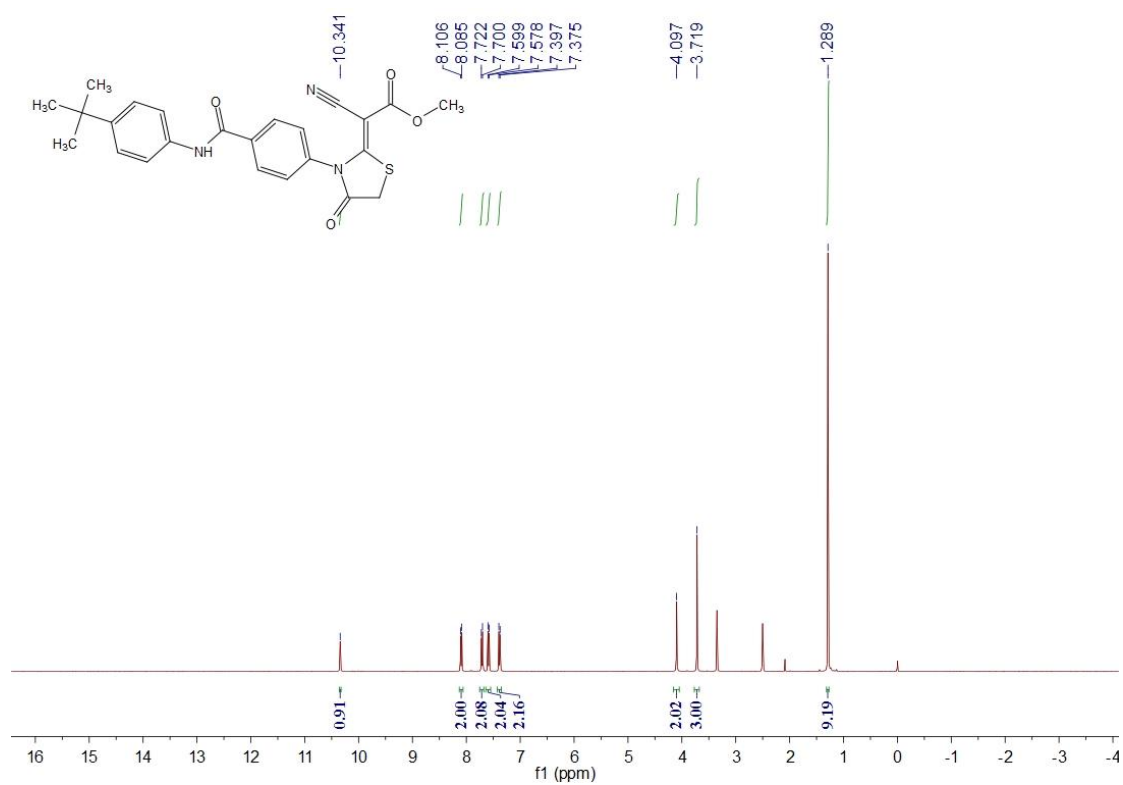
FigureS68. ^{13}C -NMR of compound 35.



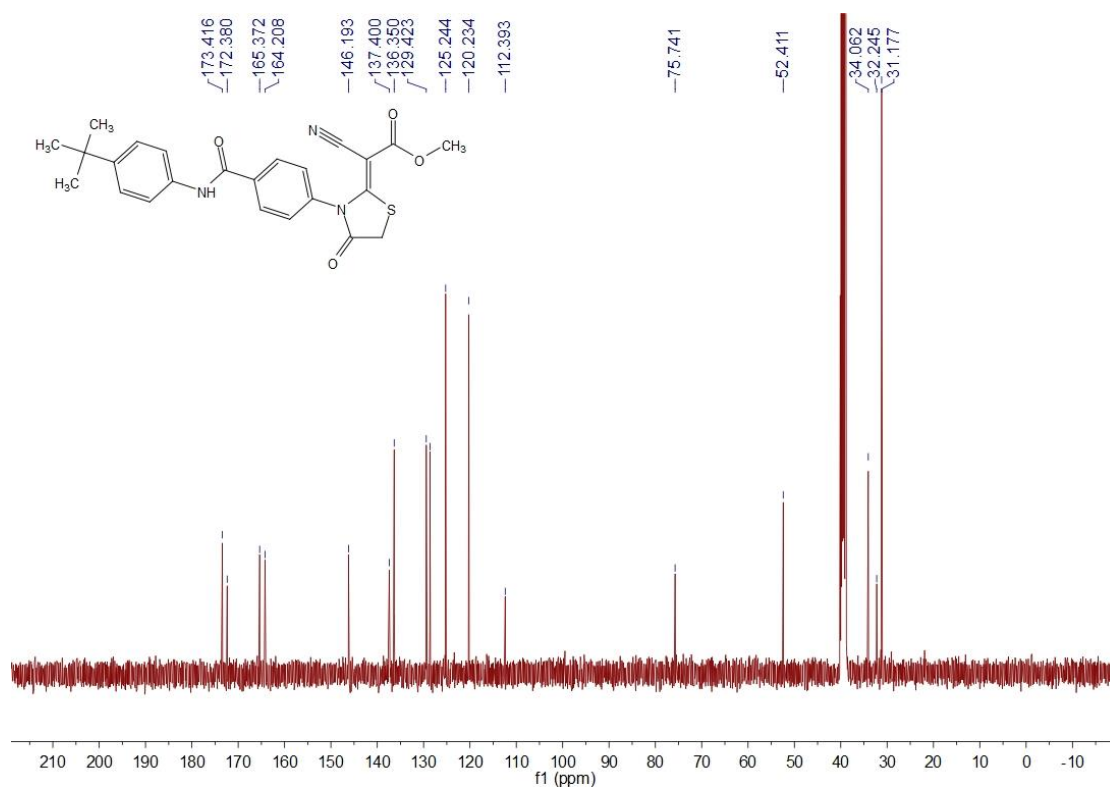
FigureS69. ¹H-NMR of compound 36.



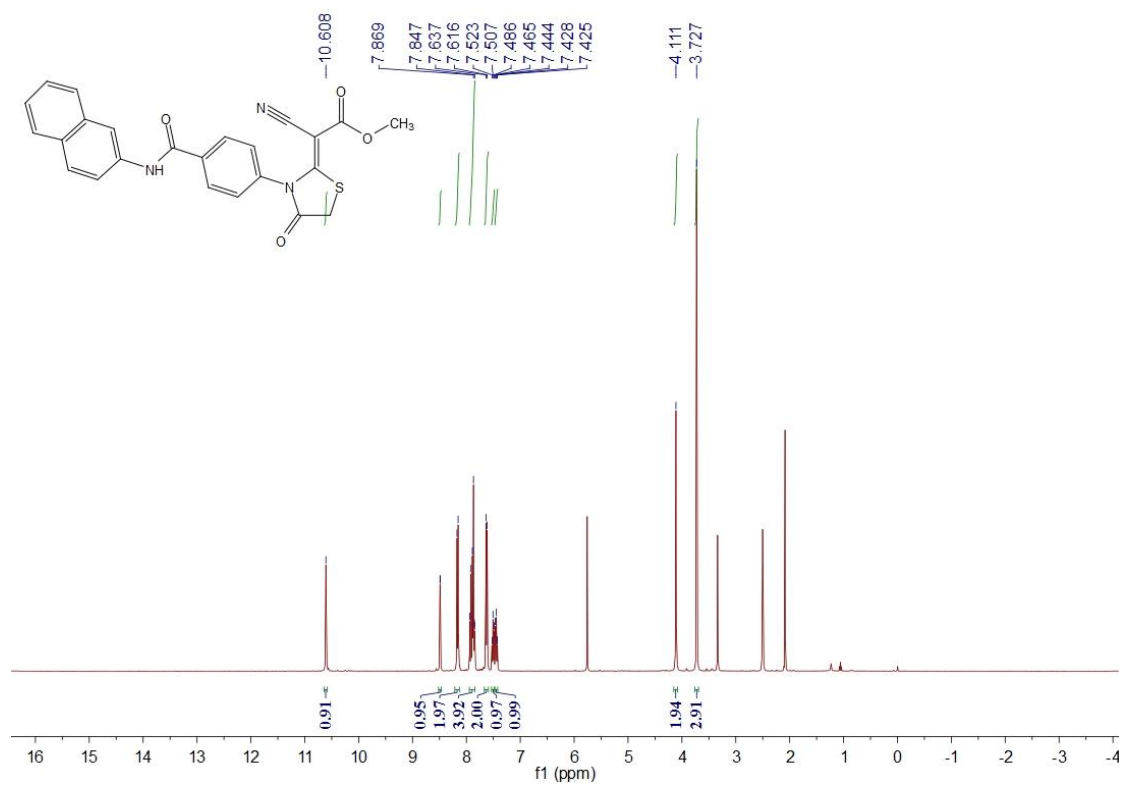
FigureS70. ¹³C-NMR of compound 36



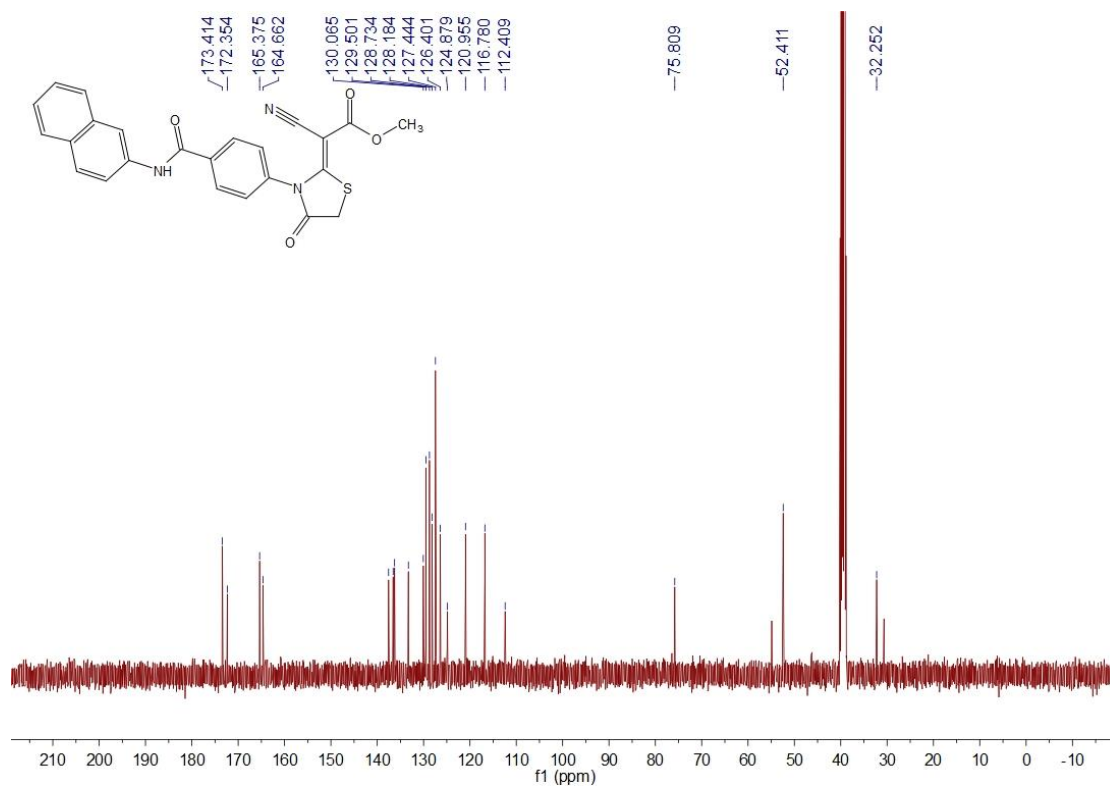
FigureS71. ¹H-NMR of compound 37.



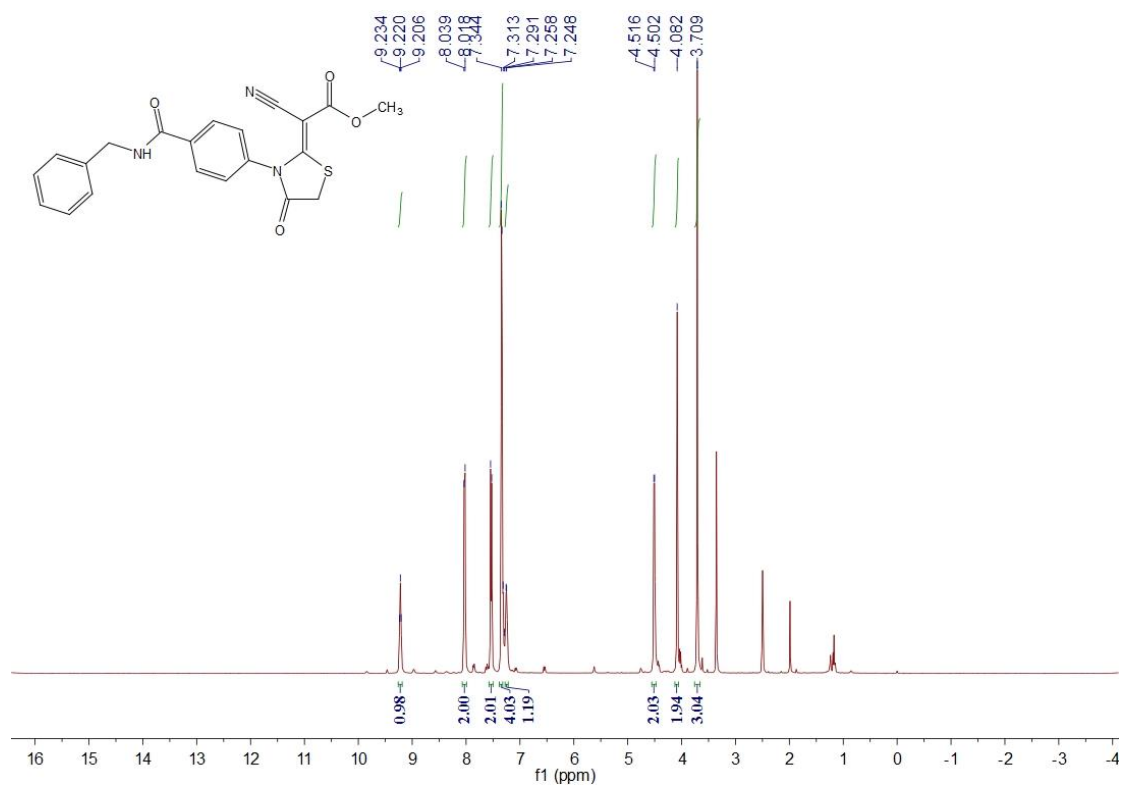
FigureS72. ¹³C-NMR of compound 37.



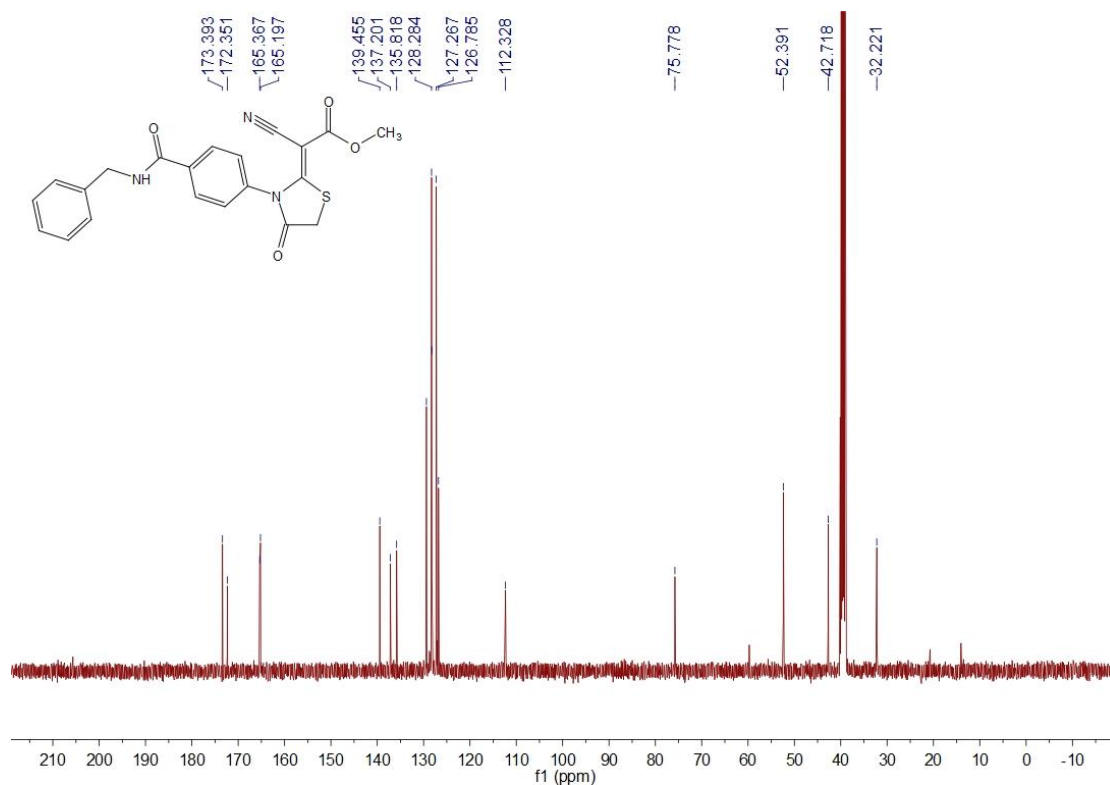
FigureS73. ¹H-NMR of compound 38.



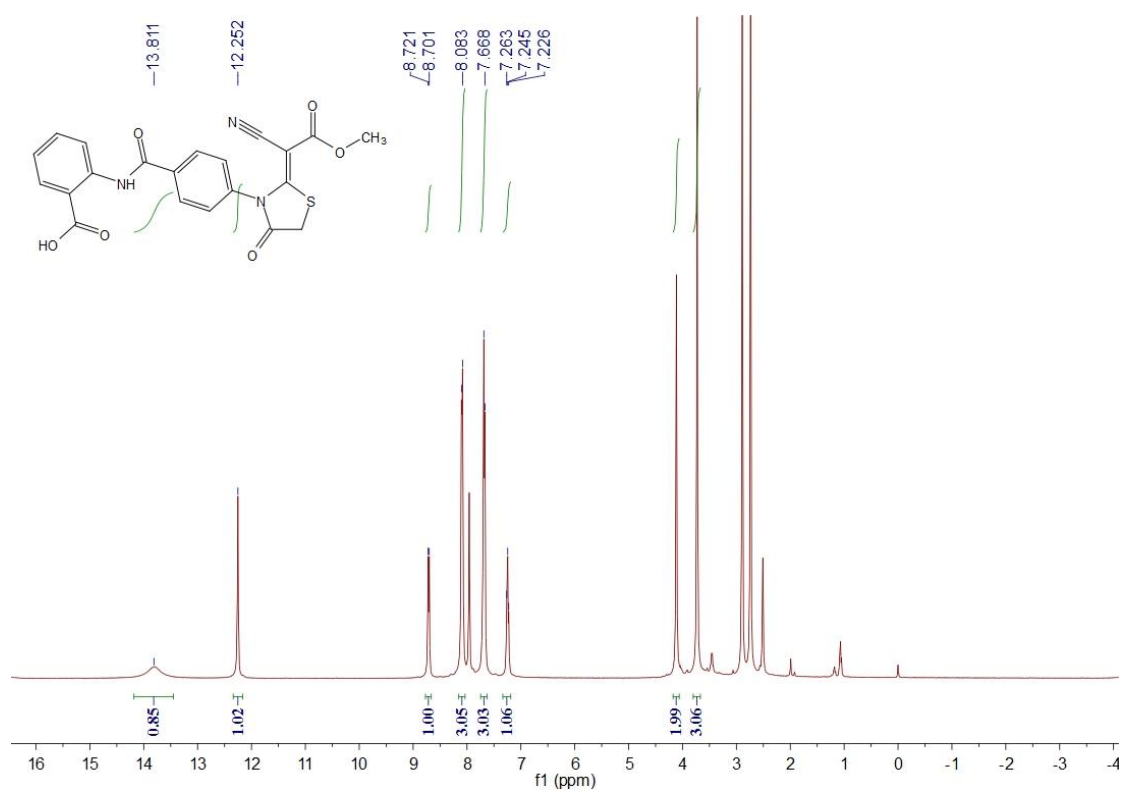
FigureS74. ¹³C-NMR of compound 38.



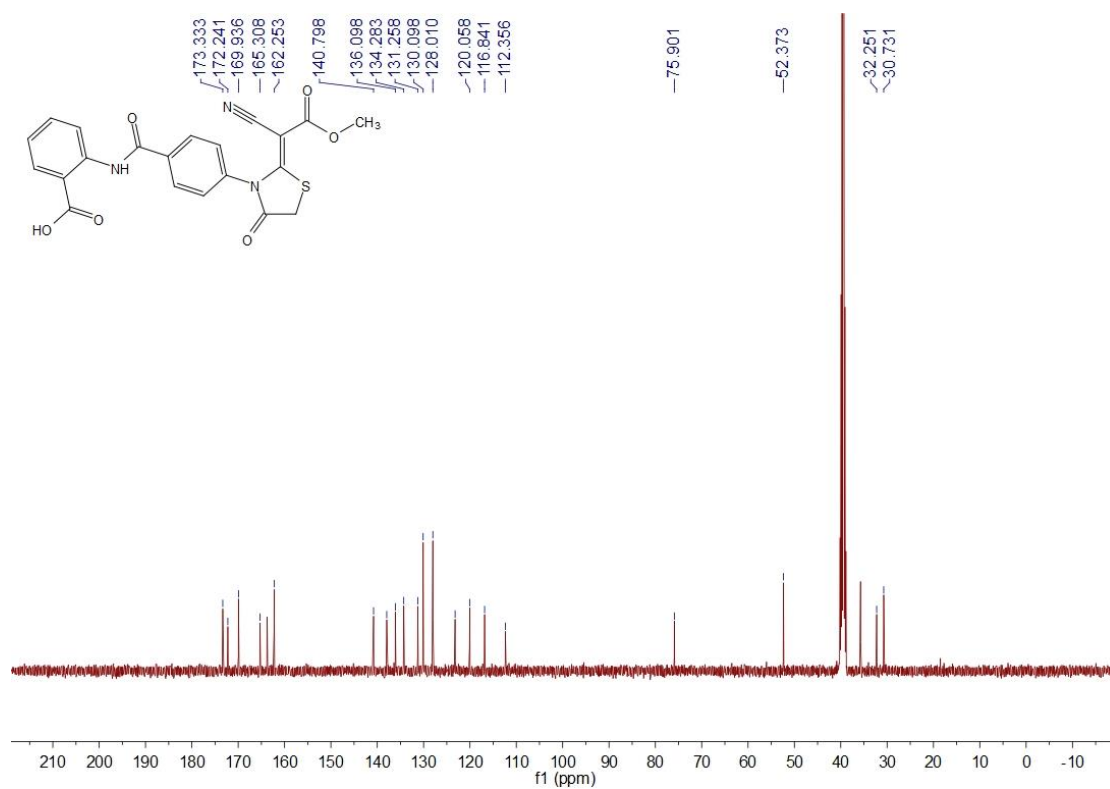
FigureS75. ¹H-NMR of compound 39.



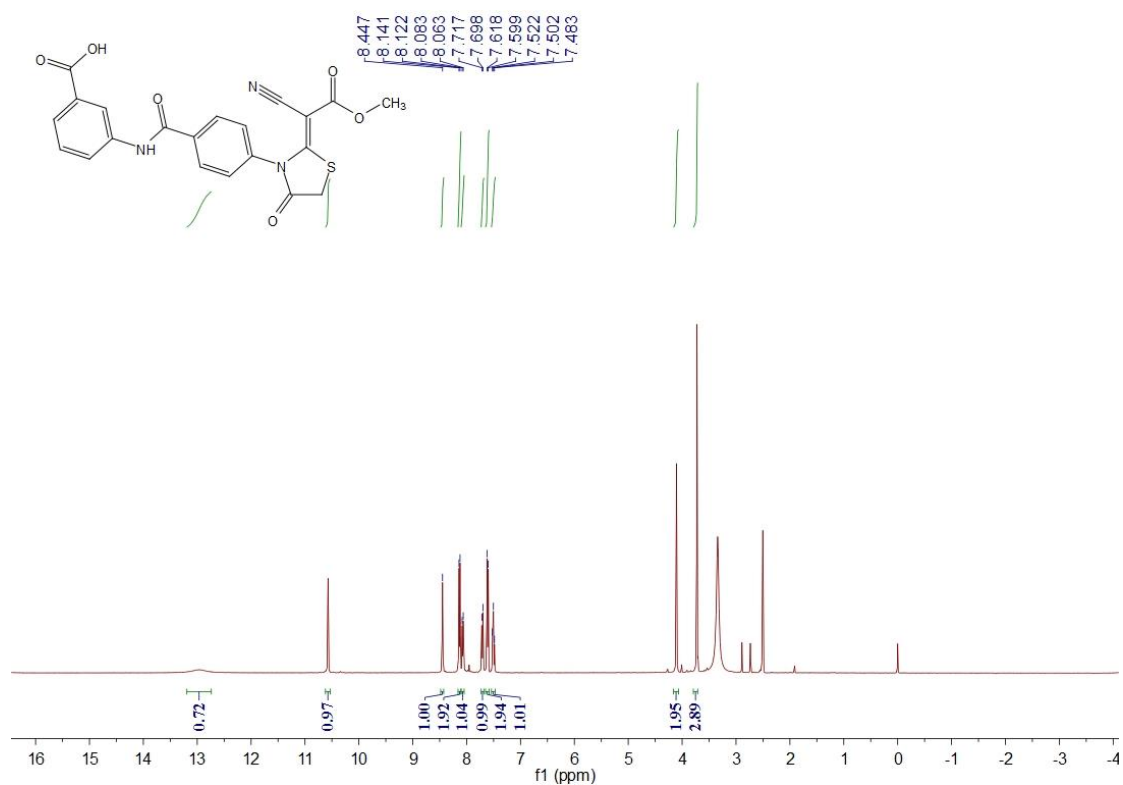
FigureS76. ¹³C-NMR of compound 39.



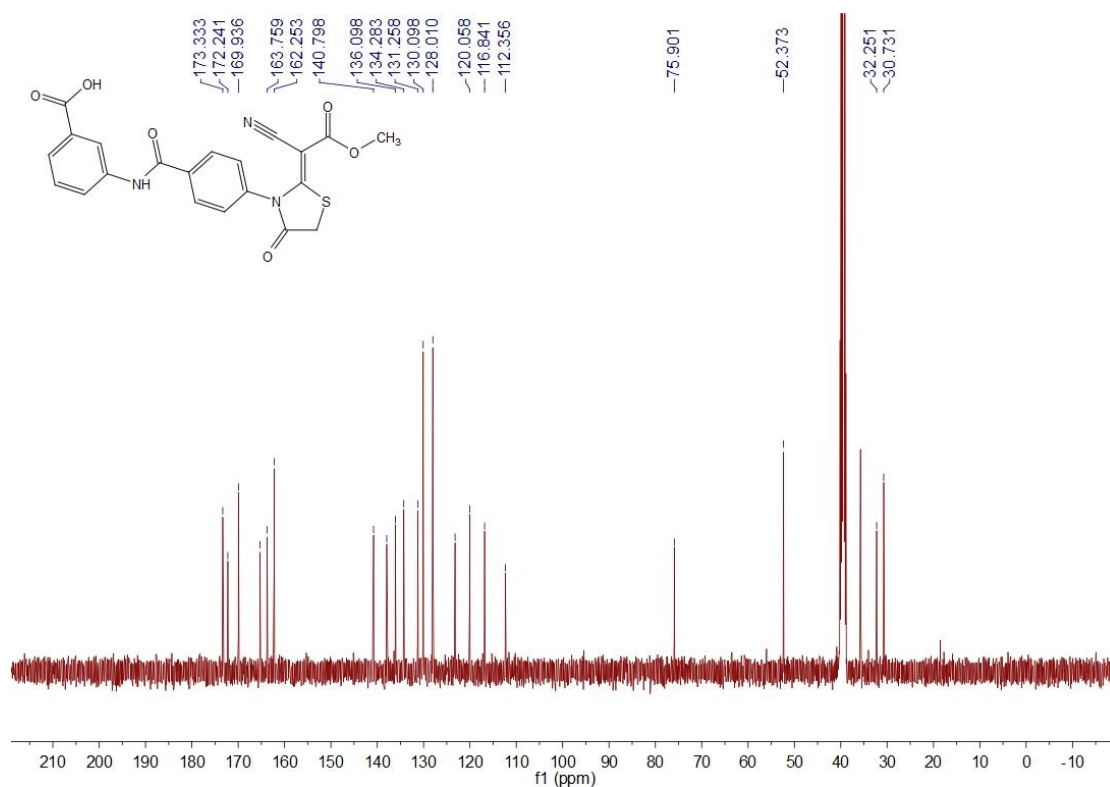
FigureS77. ^1H -NMR of compound 40.



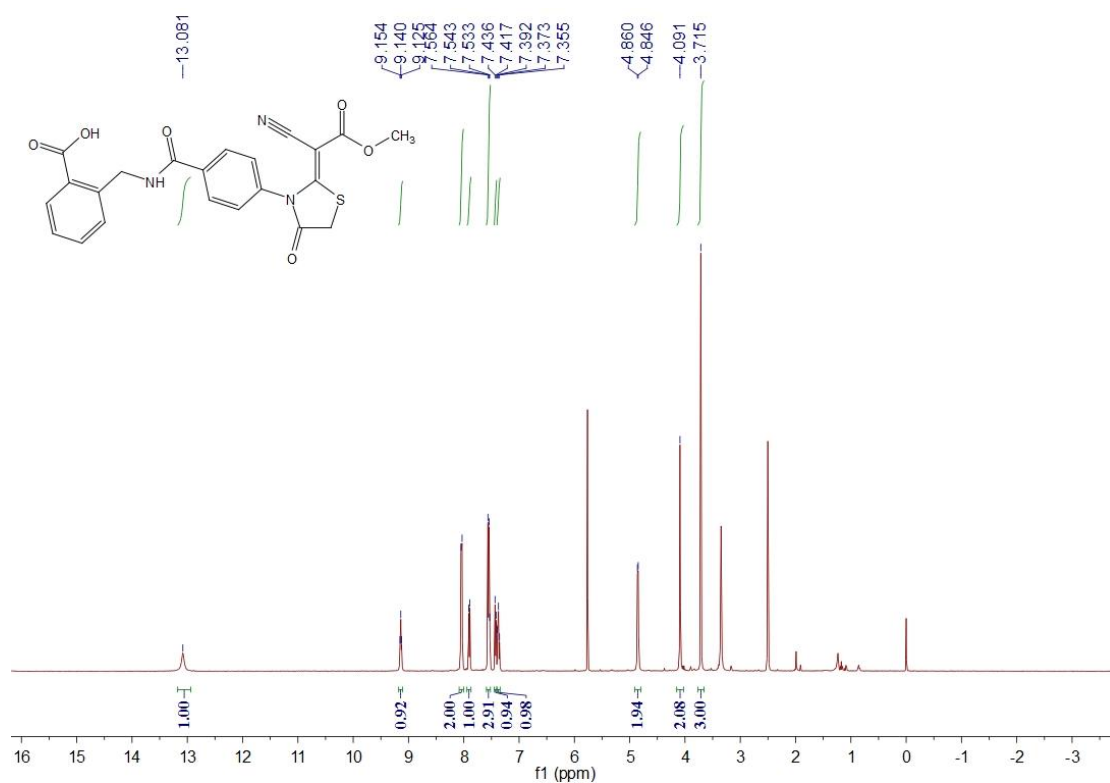
FigureS78. ^{13}C -NMR of compound 40.



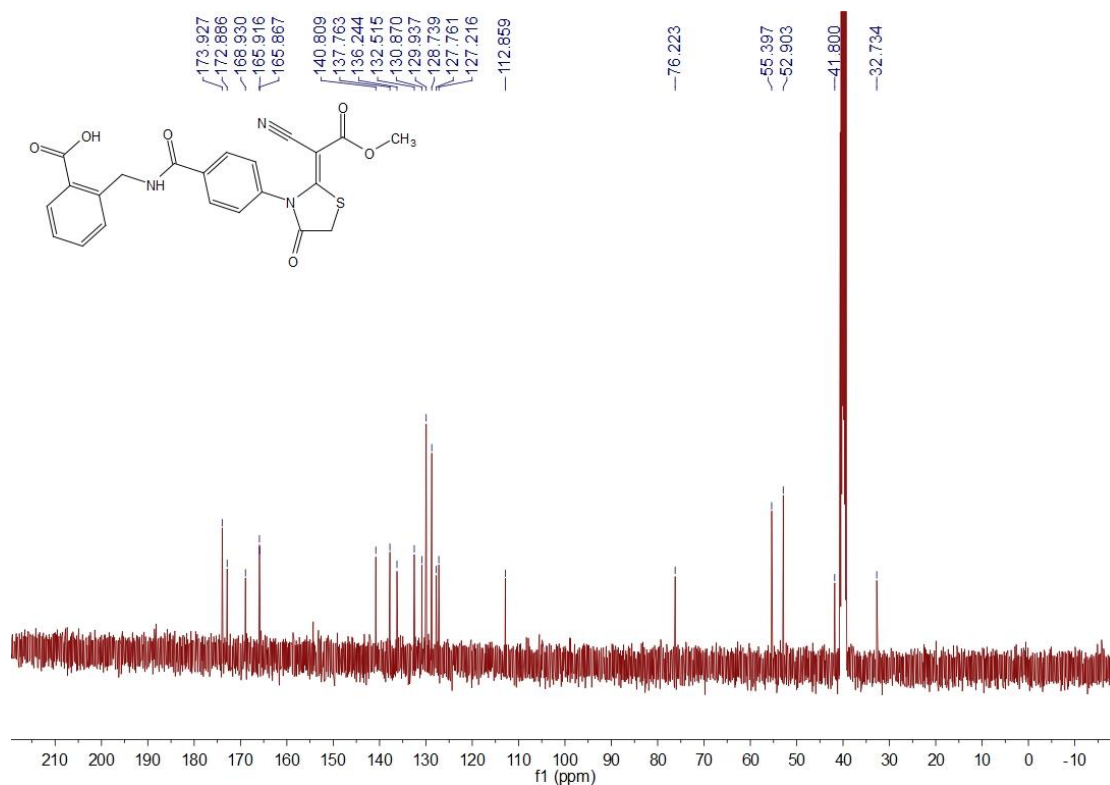
FigureS79.¹H-NMR of compound **41**.



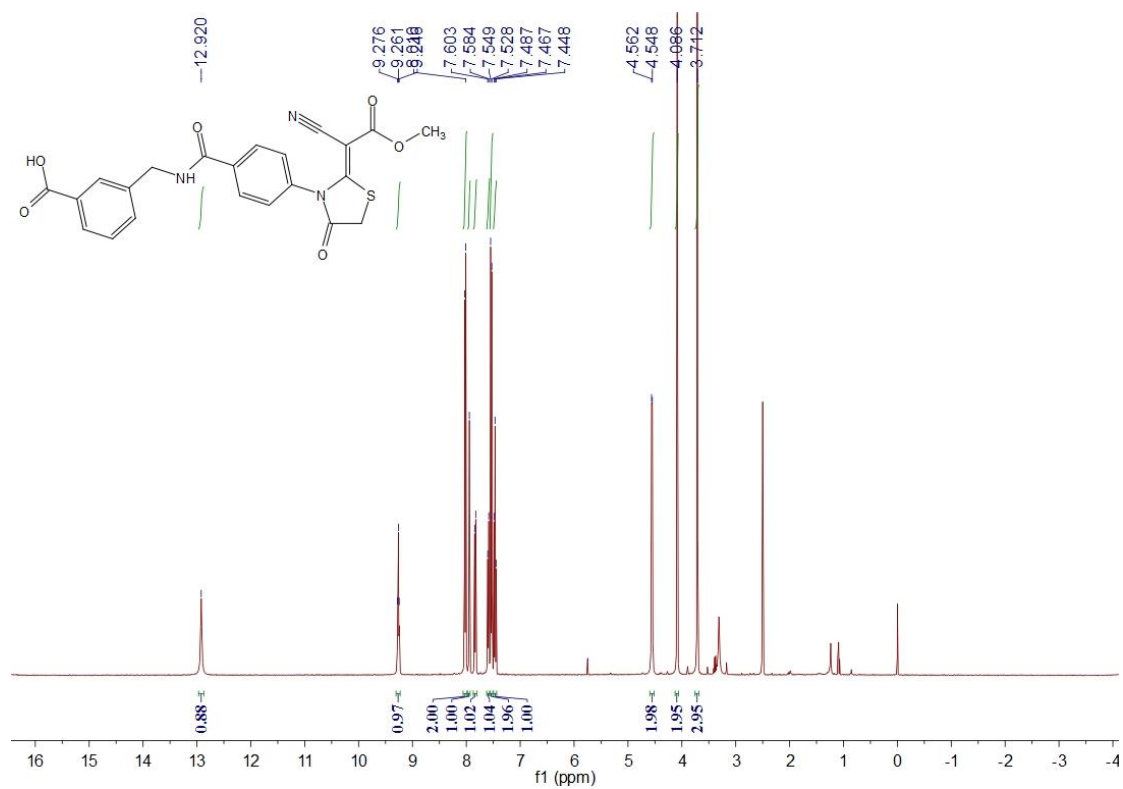
FigureS80.¹³C-NMR of compound **41**.



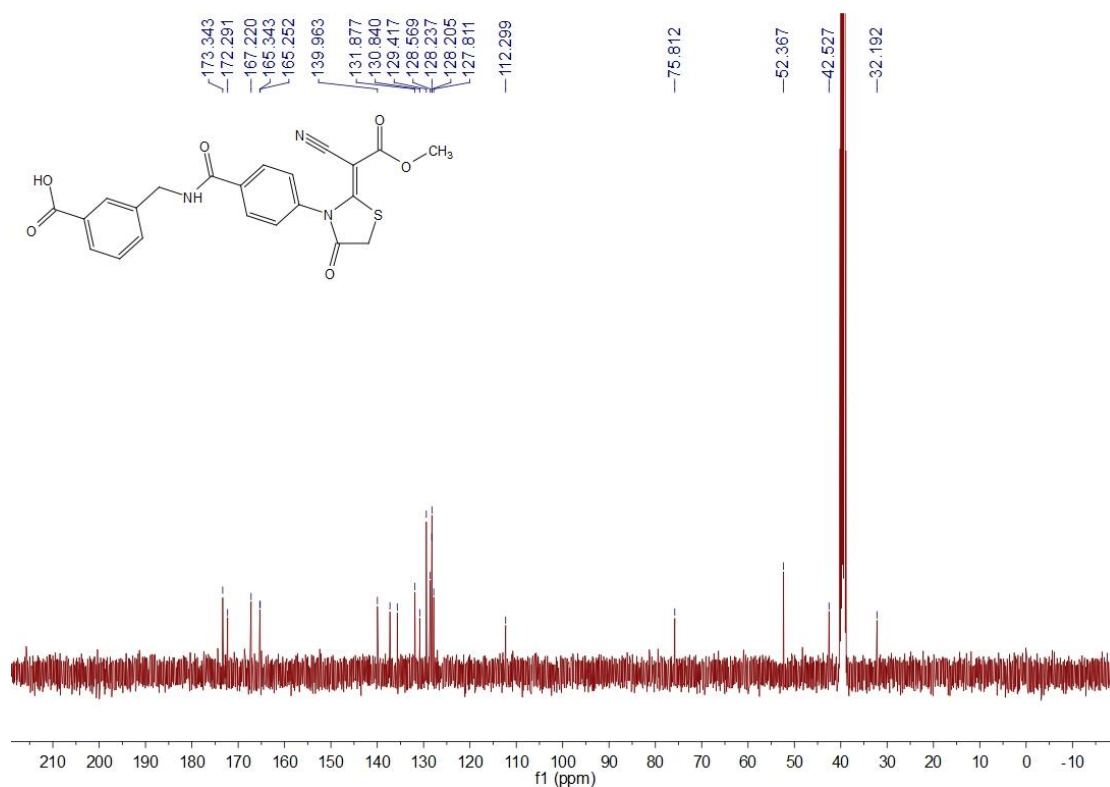
FigureS81.¹H-NMR of compound 42.



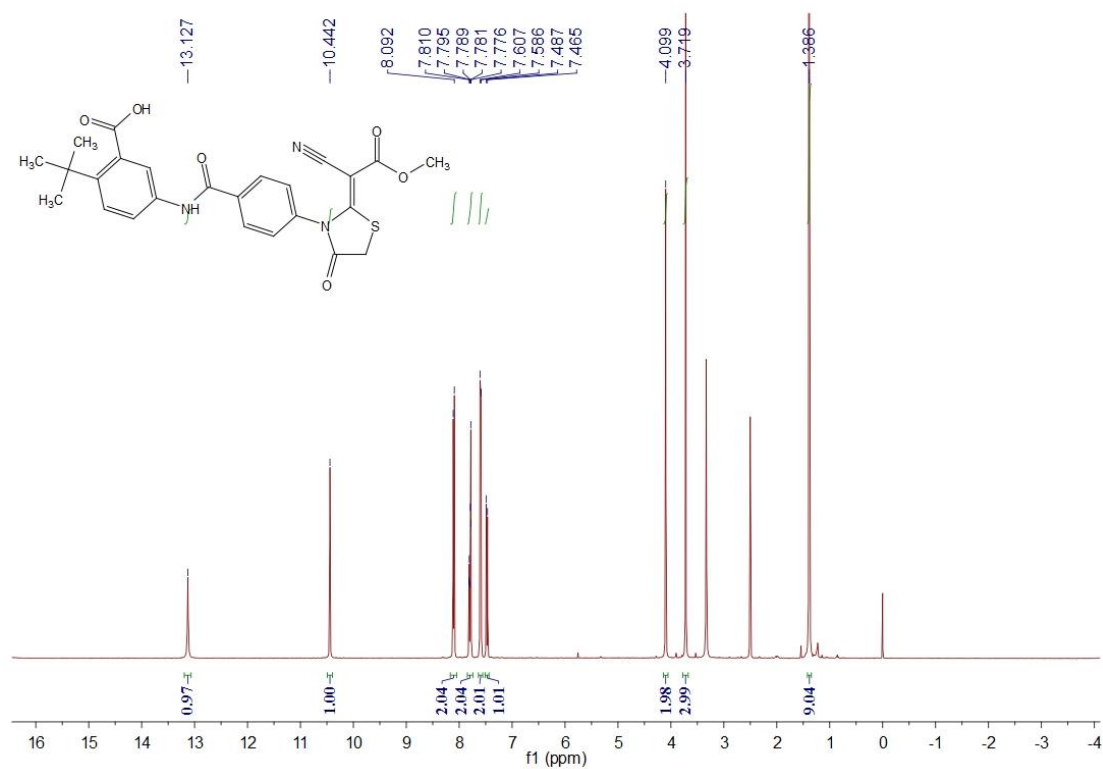
FigureS82.¹³C-NMR of compound 42.



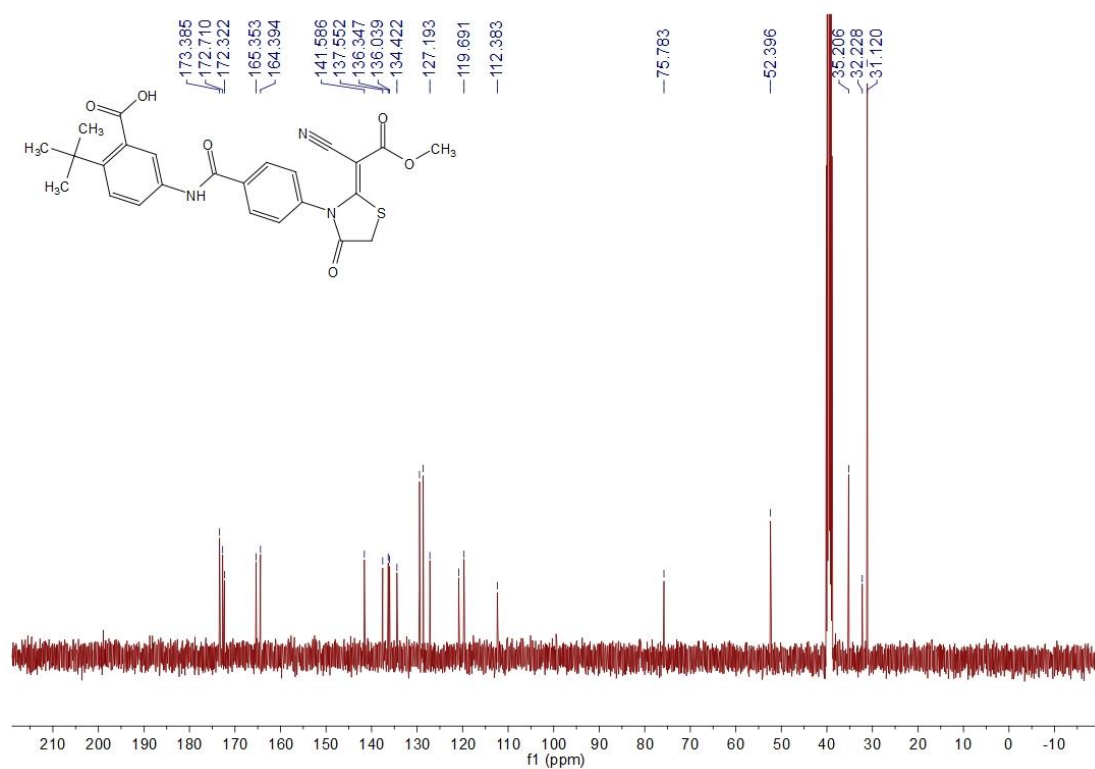
FigureS83. ¹H-NMR of compound 43.



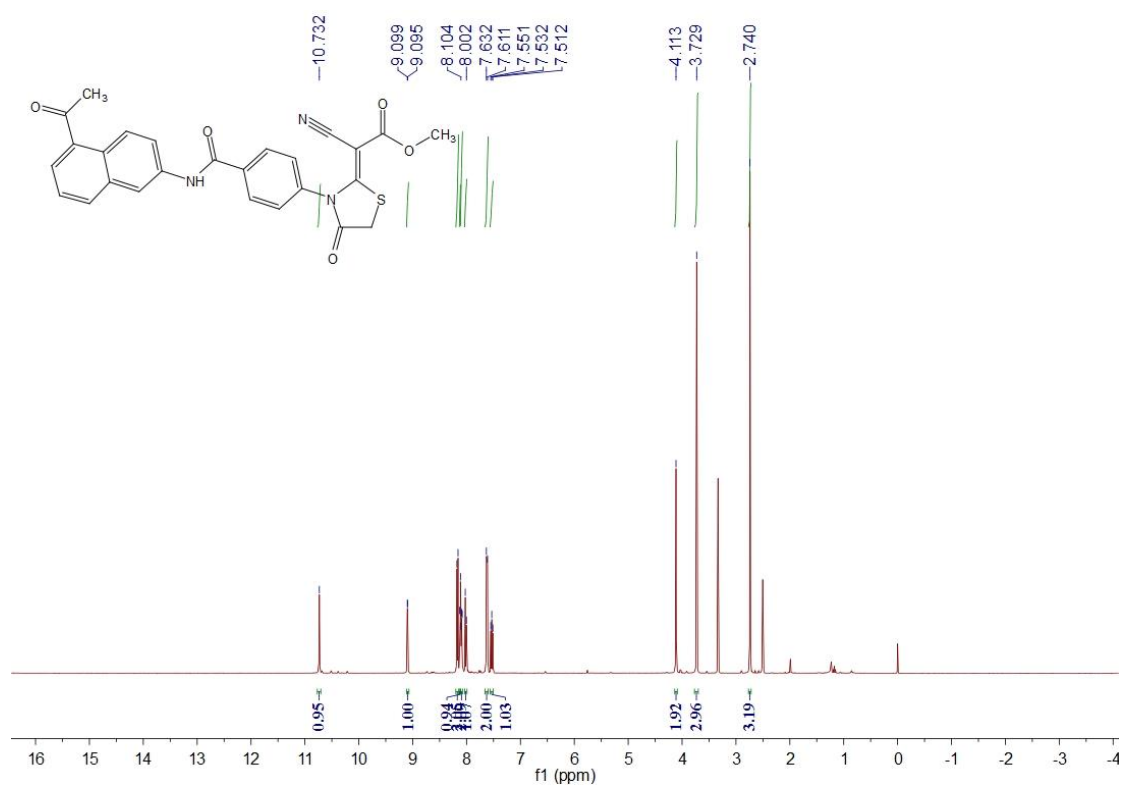
FigureS84. ¹³C-NMR of compound 43.



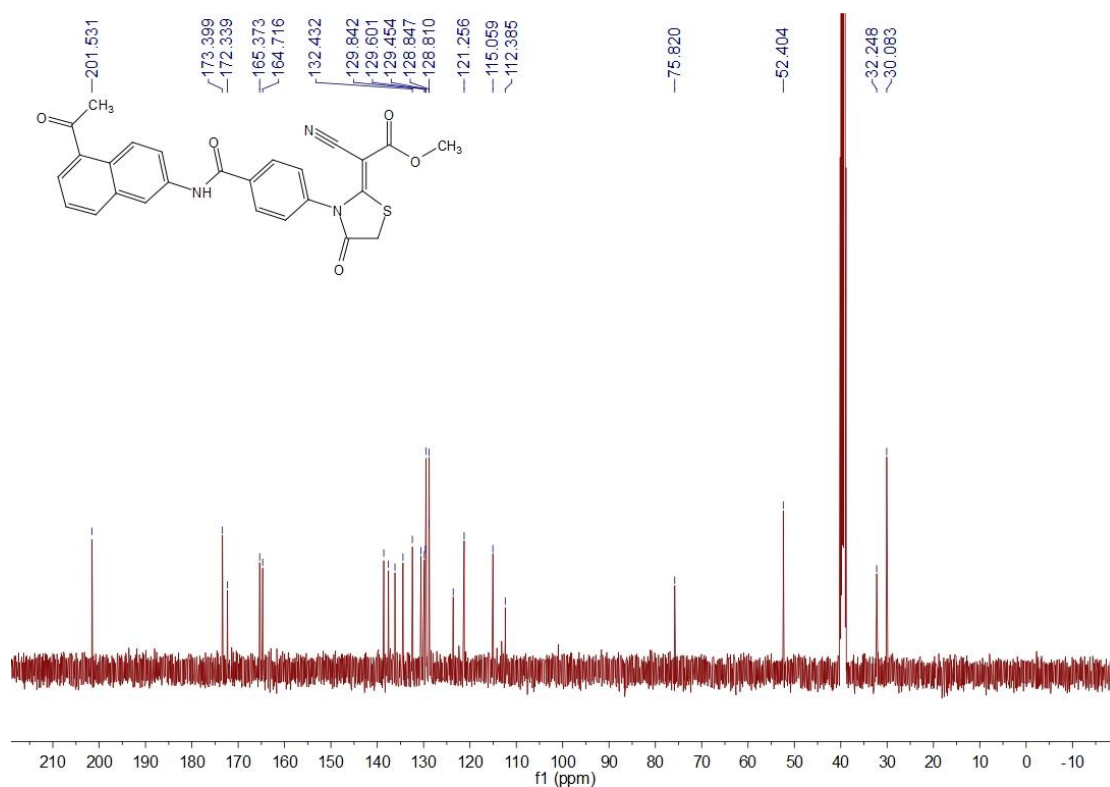
FigureS85. ¹H-NMR of compound 44.



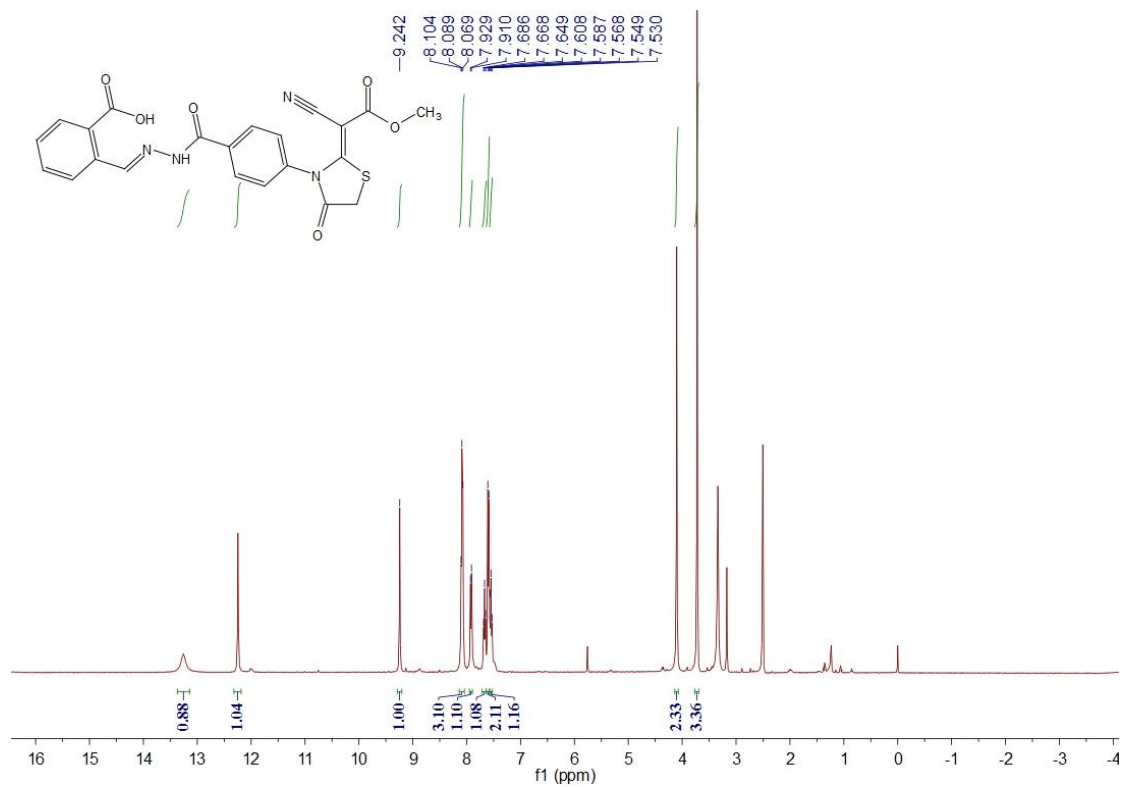
FigureS86. ¹³C-NMR of compound 44.



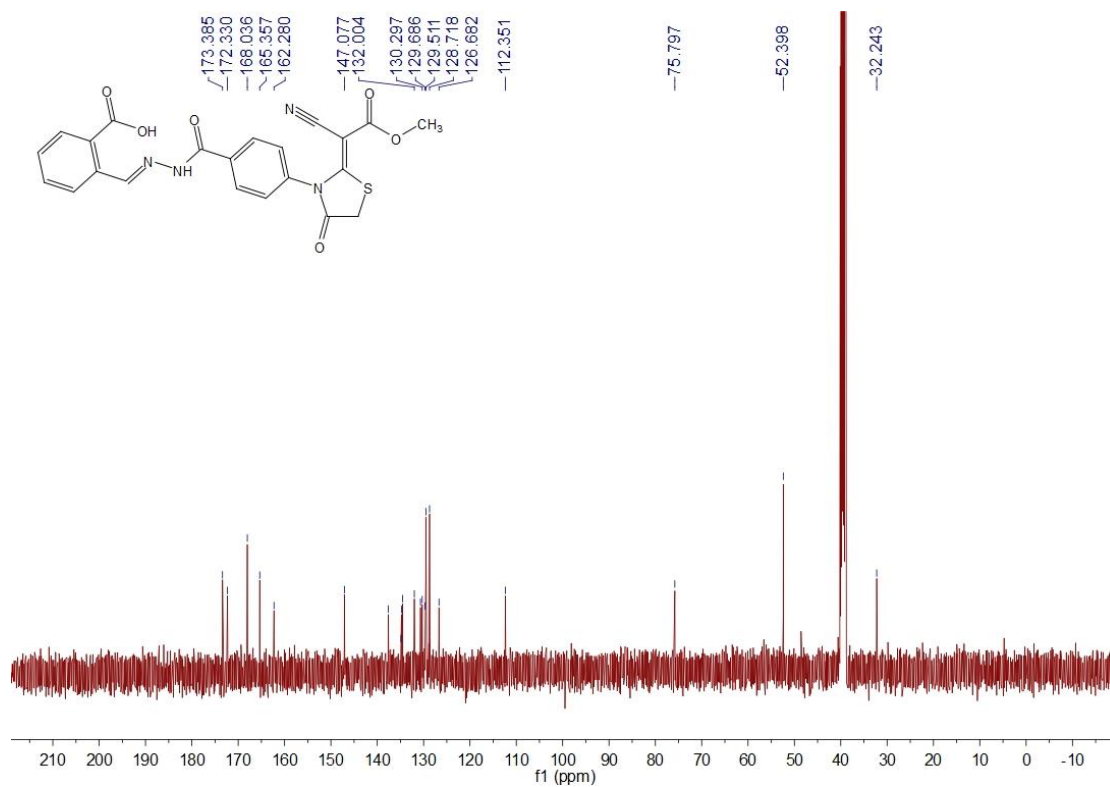
FigureS87. ¹H-NMR of compound 45.



FigureS88. ¹³C-NMR of compound 45.



FigureS89. ¹H-NMR of compound 46.



FigureS90. ¹³C-NMR of compound 46.