Supporting information

Design, Synthesis, Antifungal Evaluation and Molecular Docking of Novel 1,2,4-Triazole Derivatives Containing Oxime Ether and Cyclopropyl Moieties as Potential Sterol Demethylase Inhibitors

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1 Spectrograms of target compounds 5a-5x

Compound 5a

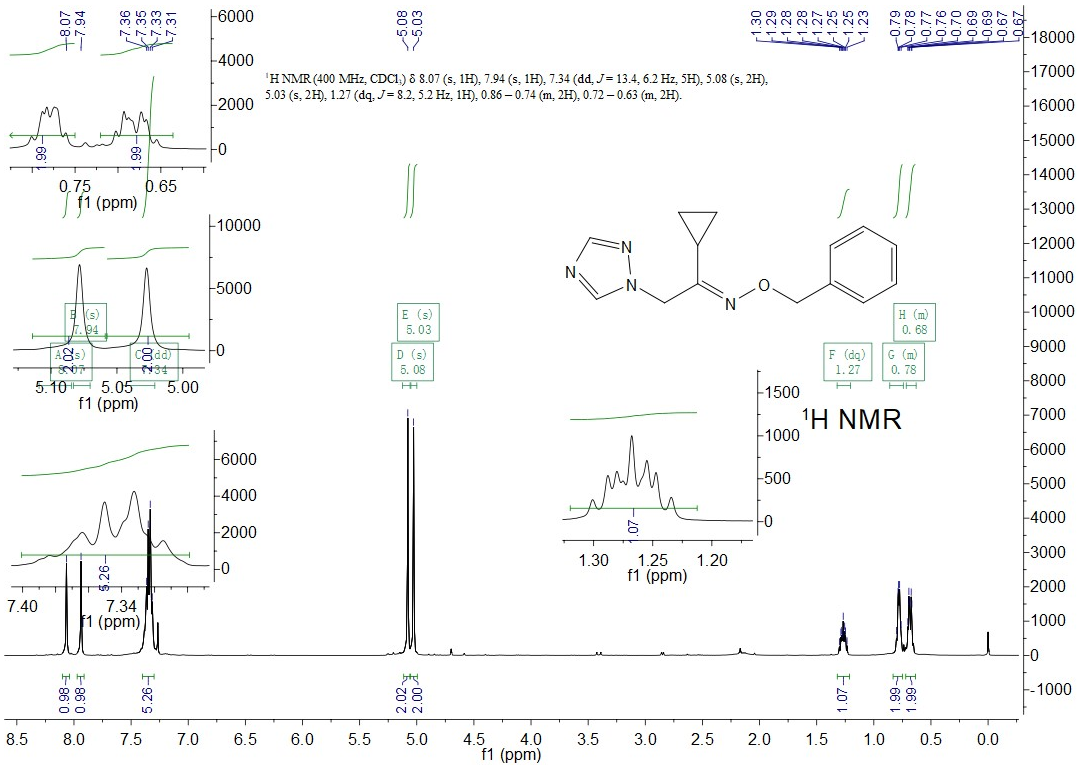

Figure 1. ^{1}H NMR sprectrum of title compound 5a

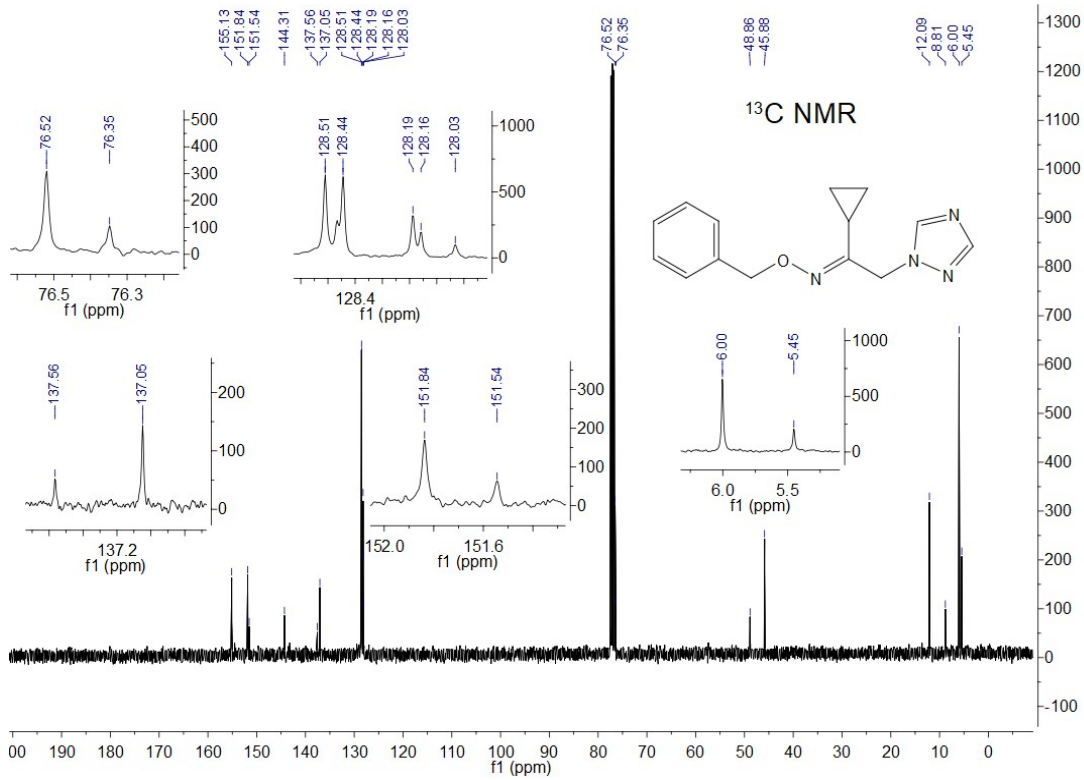

Figure 2. ^{13}C NMR sprectrum of title compound 5a

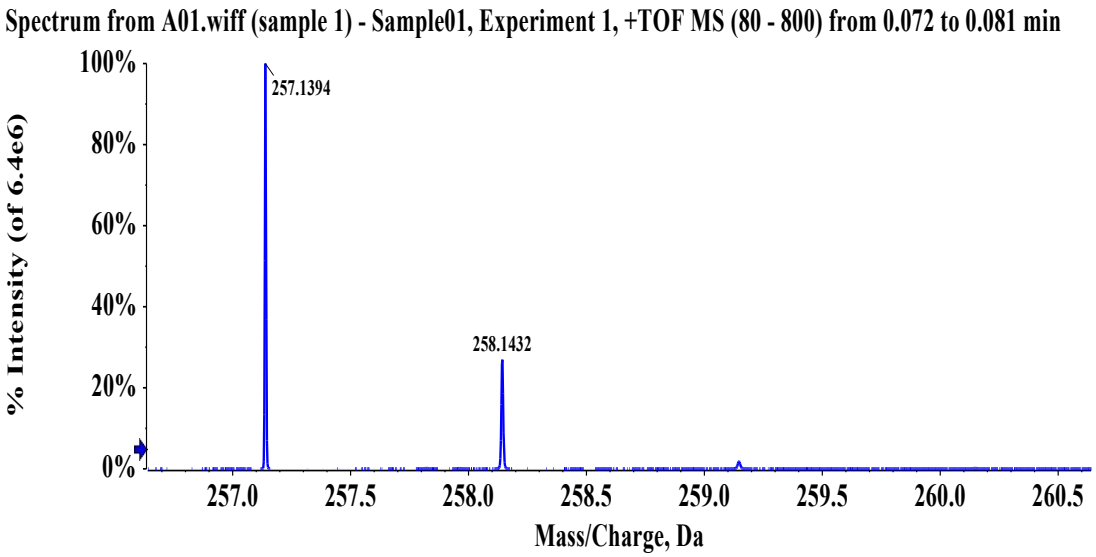

Figure 3. HRMS sprectrum of title compound 5a

Compound 5b

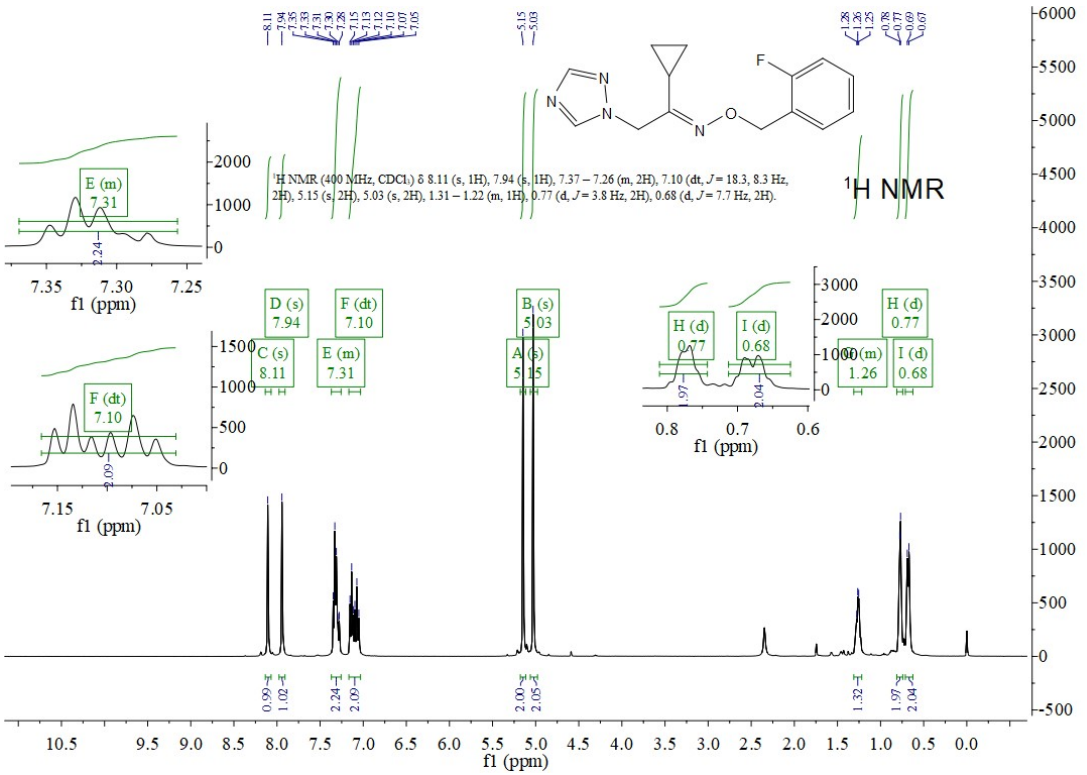

Figure 4. ^{1}H NMR sprectrum of title compound 5b

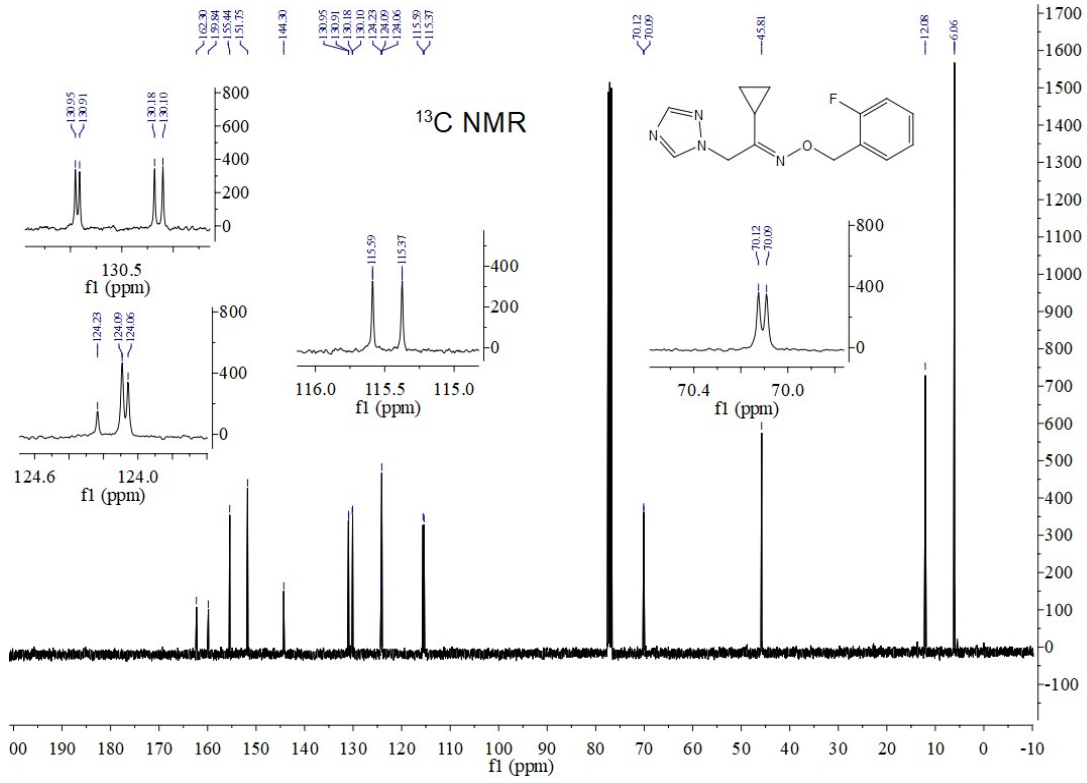

Figure 5. ^{13}C NMR sprectrum of title compound 5b

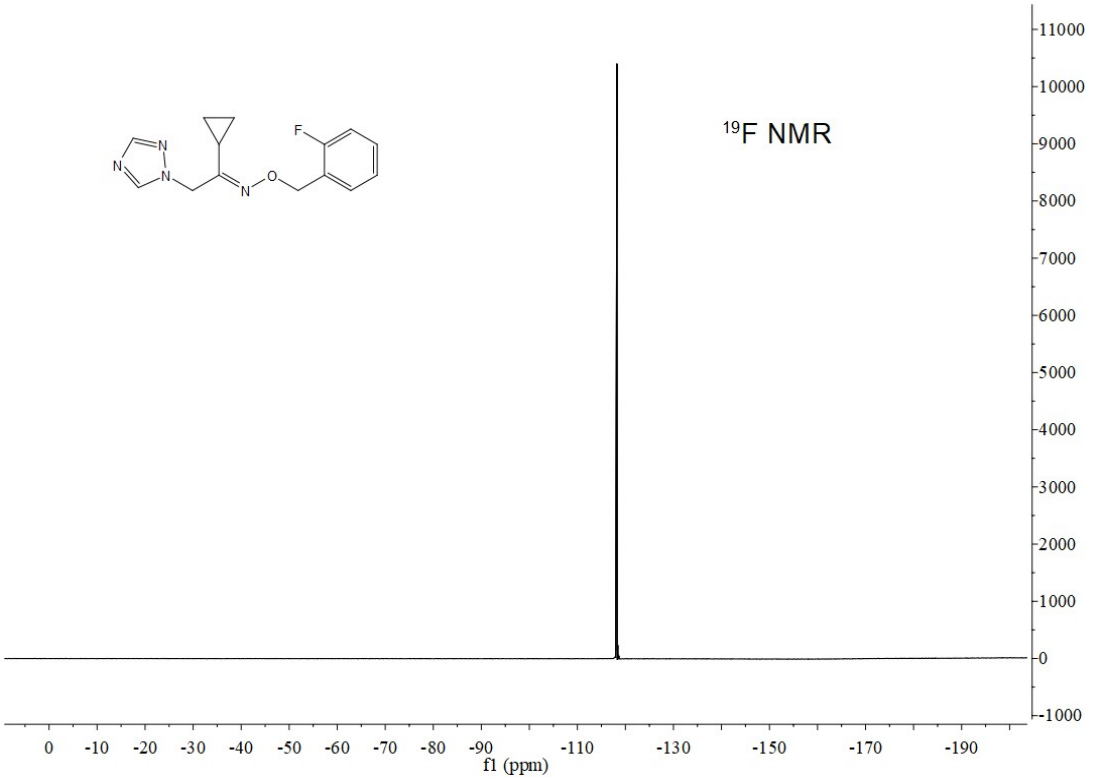

Figure 6. ^{19}F NMR sprectrum of title compound 5b

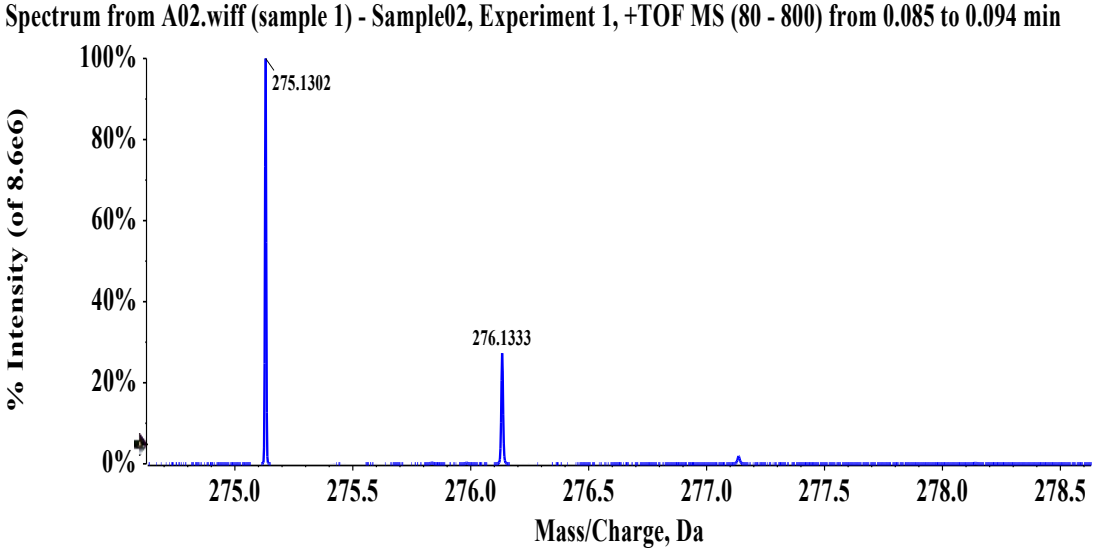

Figure 7. HRMS sprectrum of title compound 5b

Compound 5c

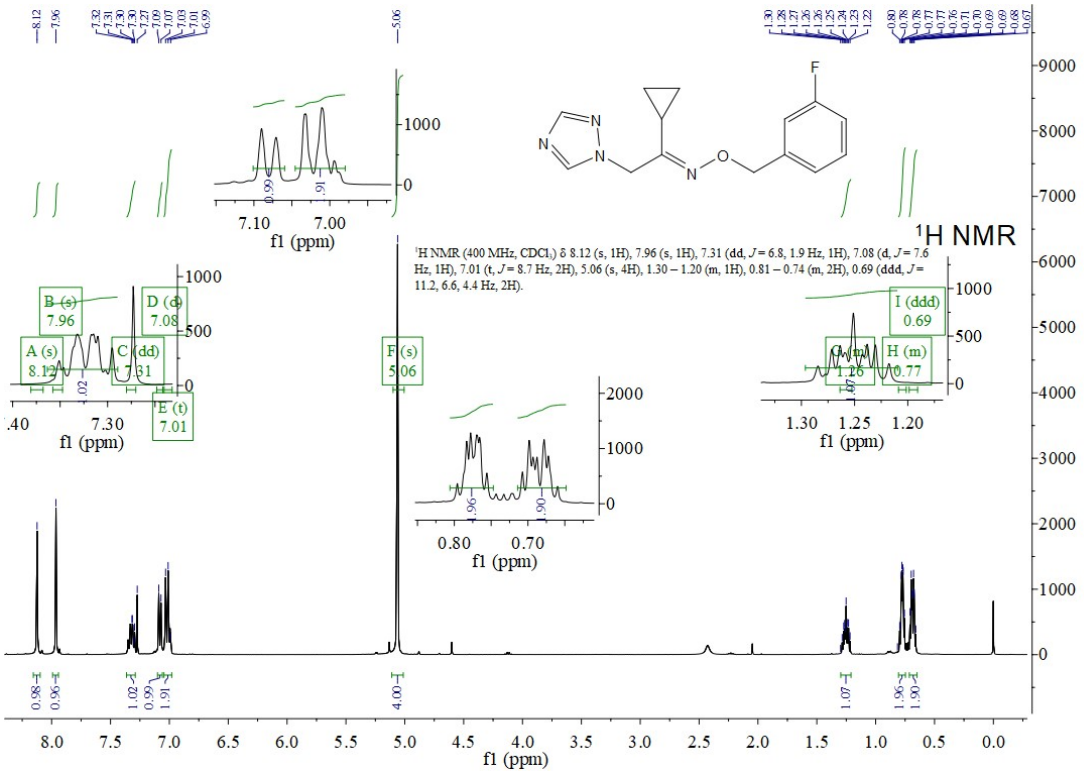

Figure 8. ^{1}H NMR sprectrum of title compound 5c

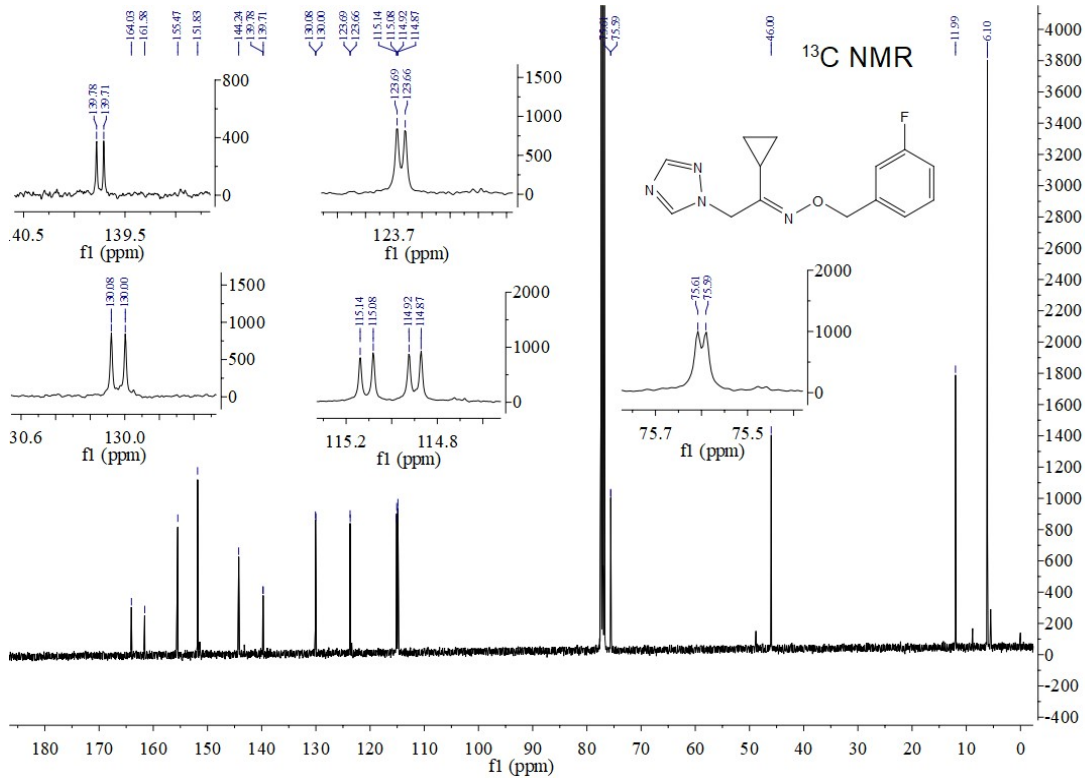

Figure 9. ^{13}C NMR sprectrum of title compound 5c

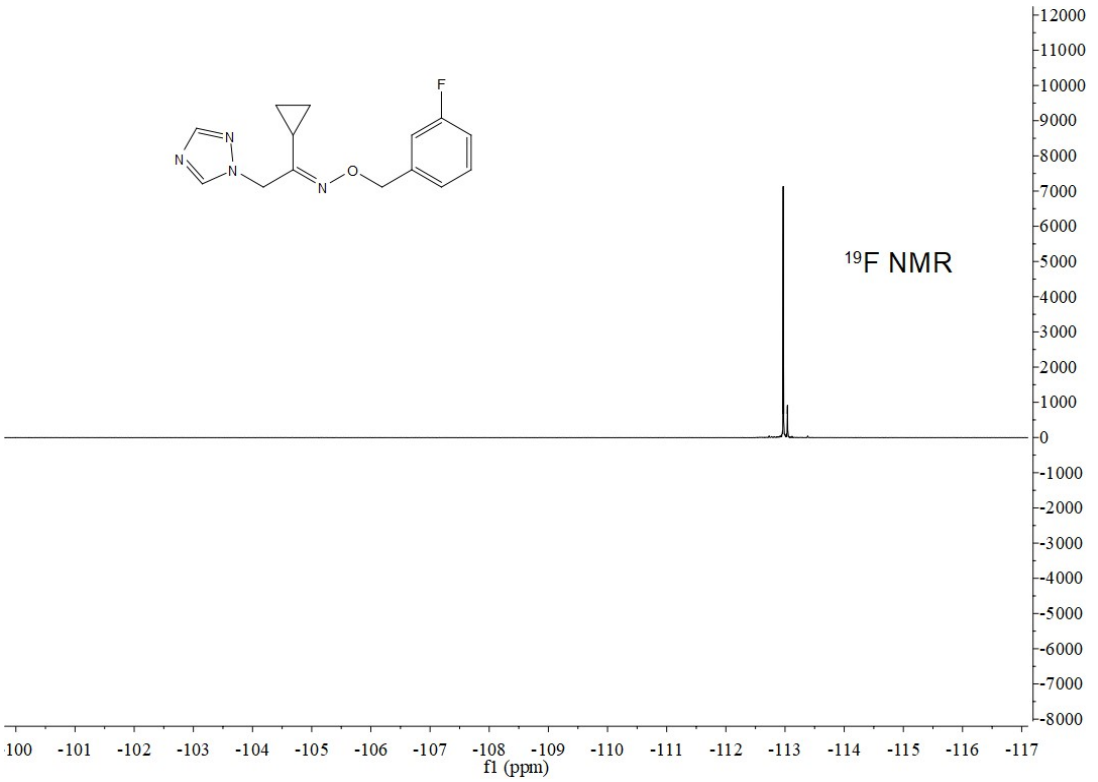

Figure 10. ^{19}F NMR sprectrum of title compound 5c

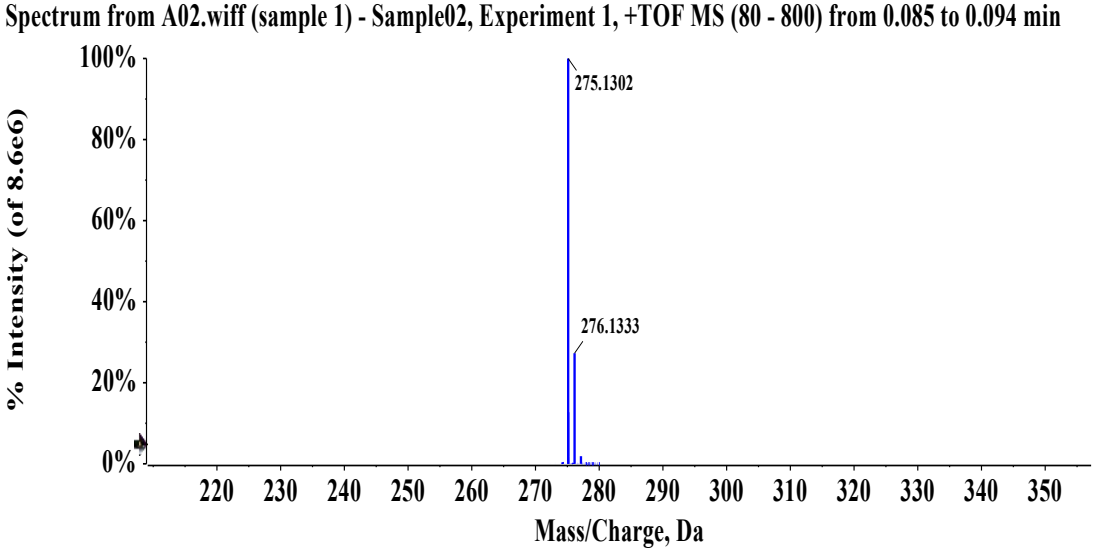

Figure 11. HRMS sprectrum of title compound 5c

Compound 5d

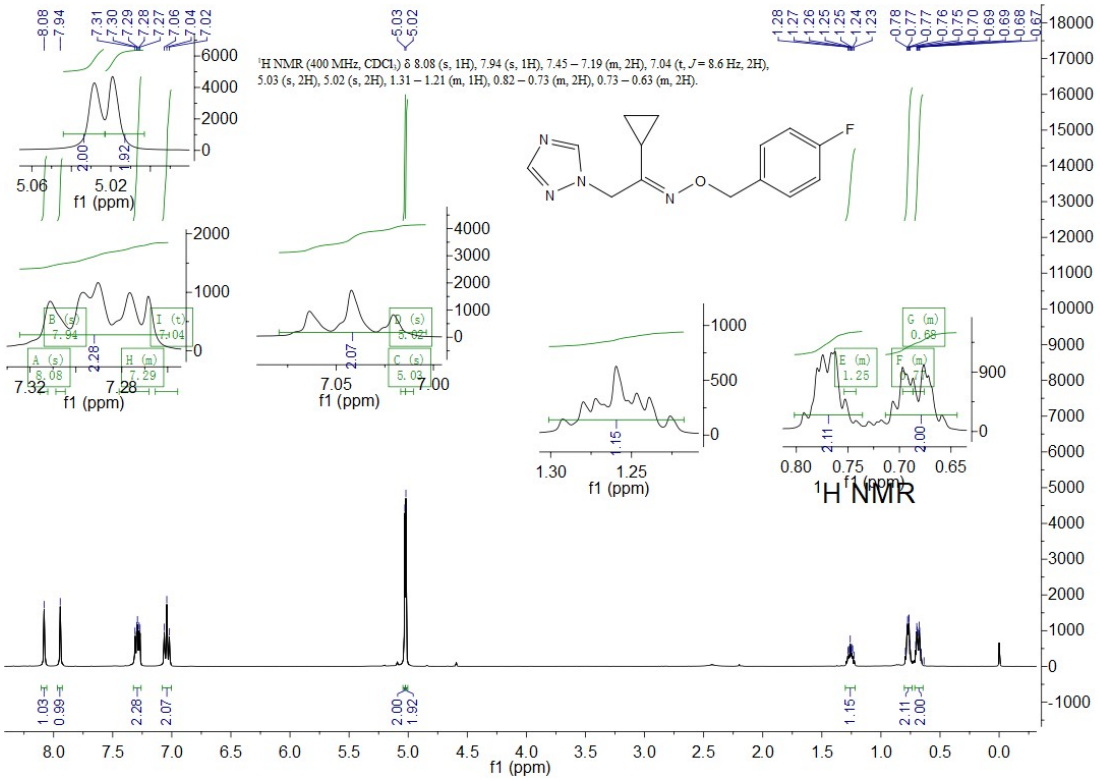

Figure 12. ^{1}H NMR sprectrum of title compound 5d

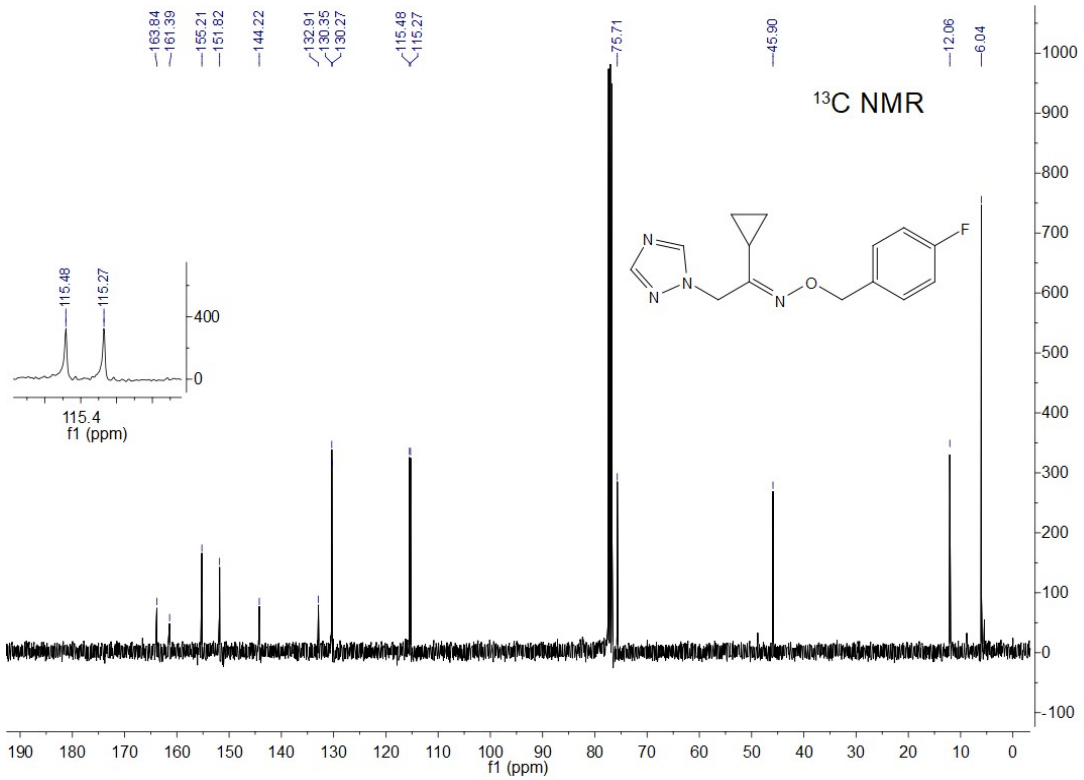

Figure 13. ^{13}C NMR sprectrum of title compound 5d

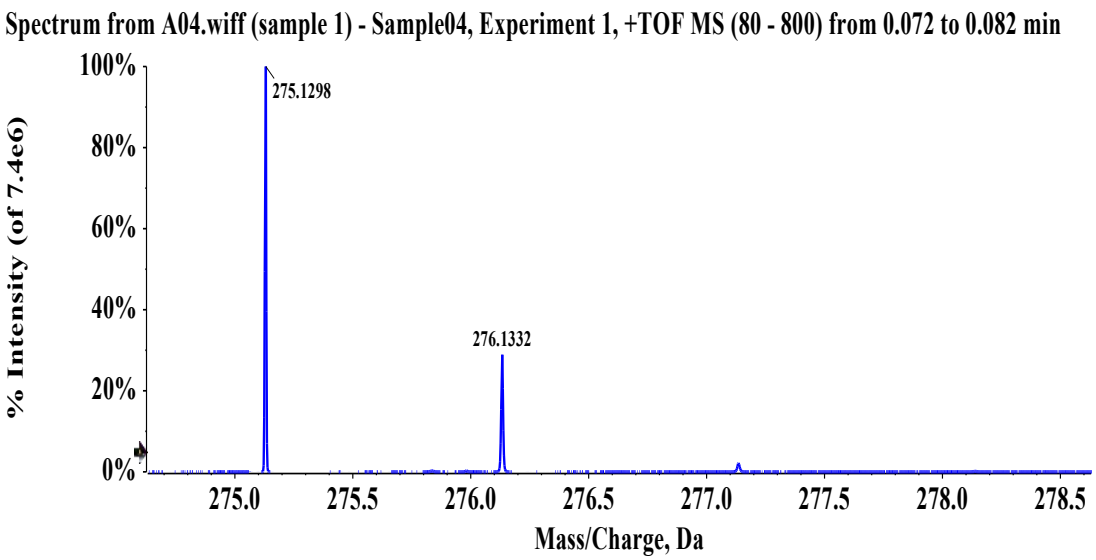

Figure 14. HRMS sprectrum of title compound 5d

Compound 5e

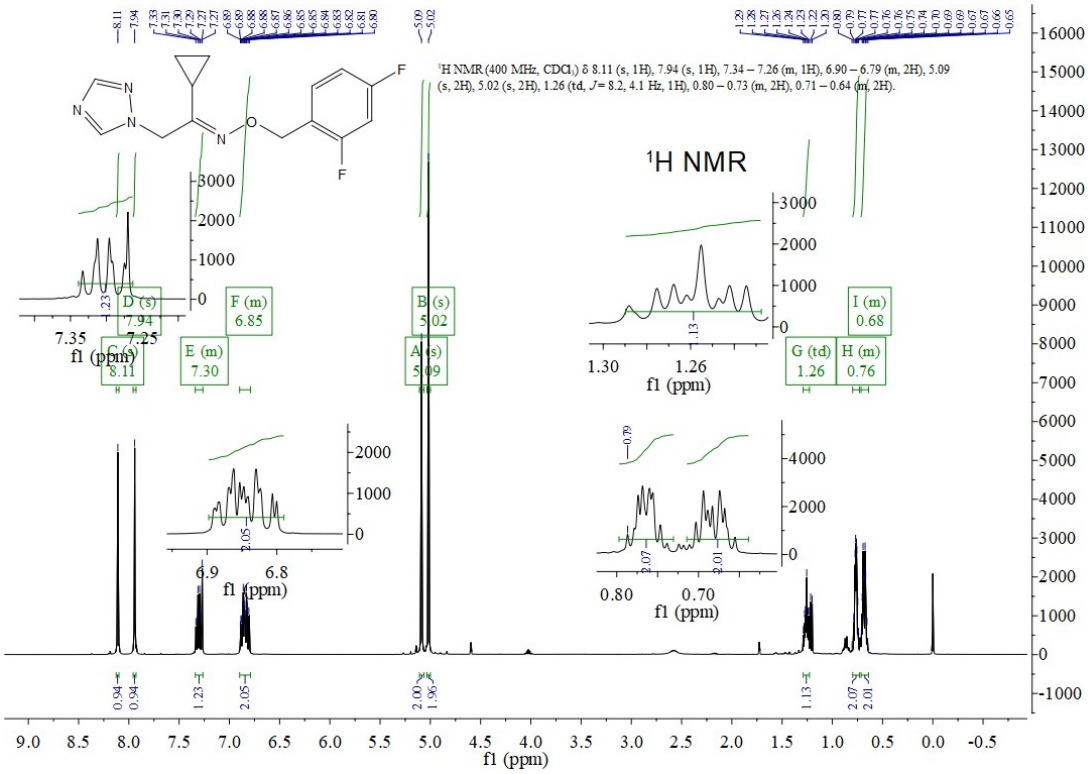

Figure 15. ^{1}H NMR sprectrum of title compound 5e

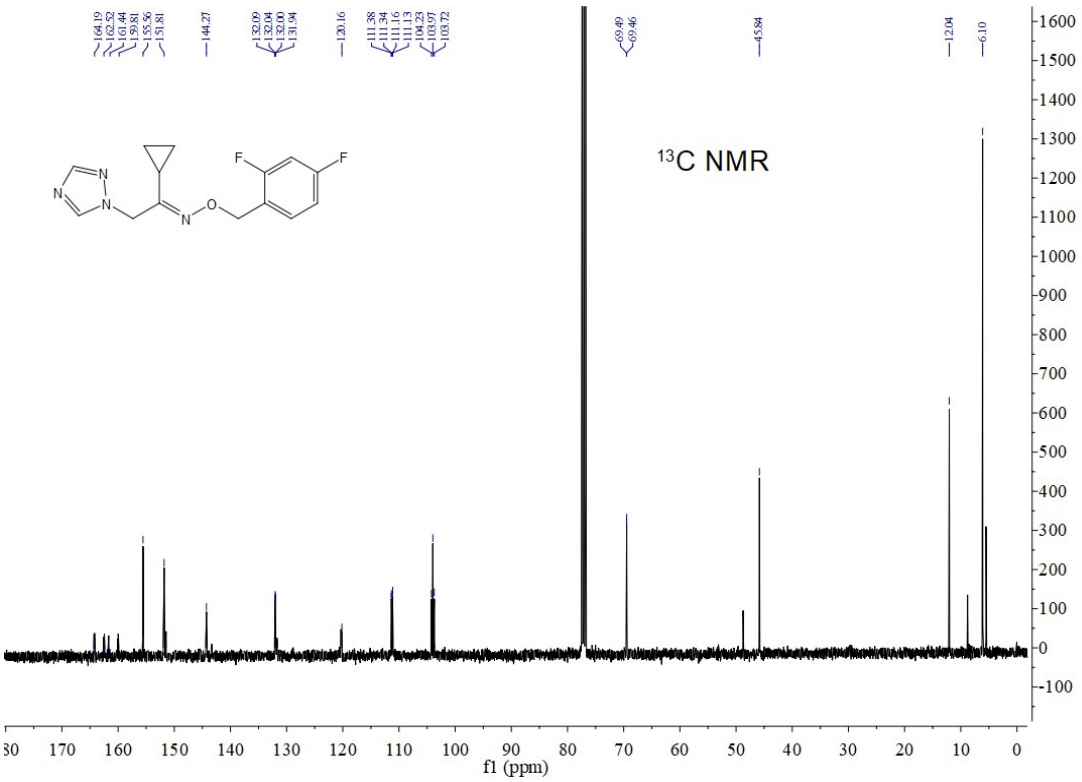

Figure 16. ^{13}C NMR sprectrum of title compound 5e

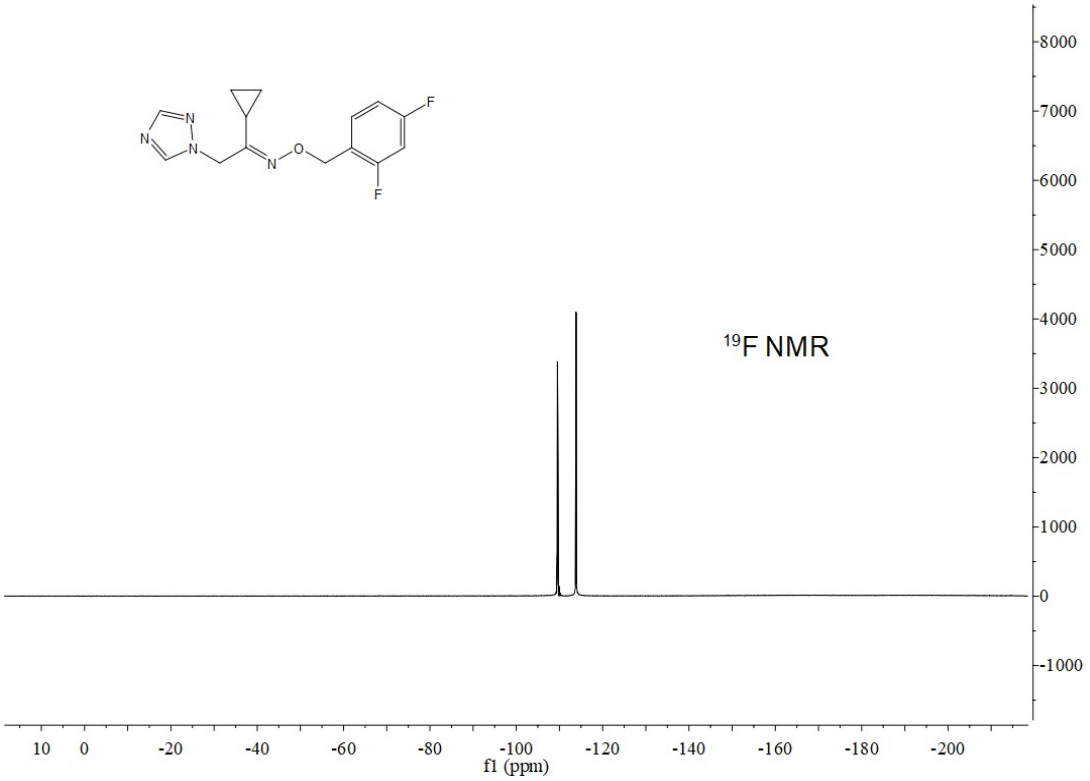

Figure 17.^{19}F NMR sprectrum of title compound 5e

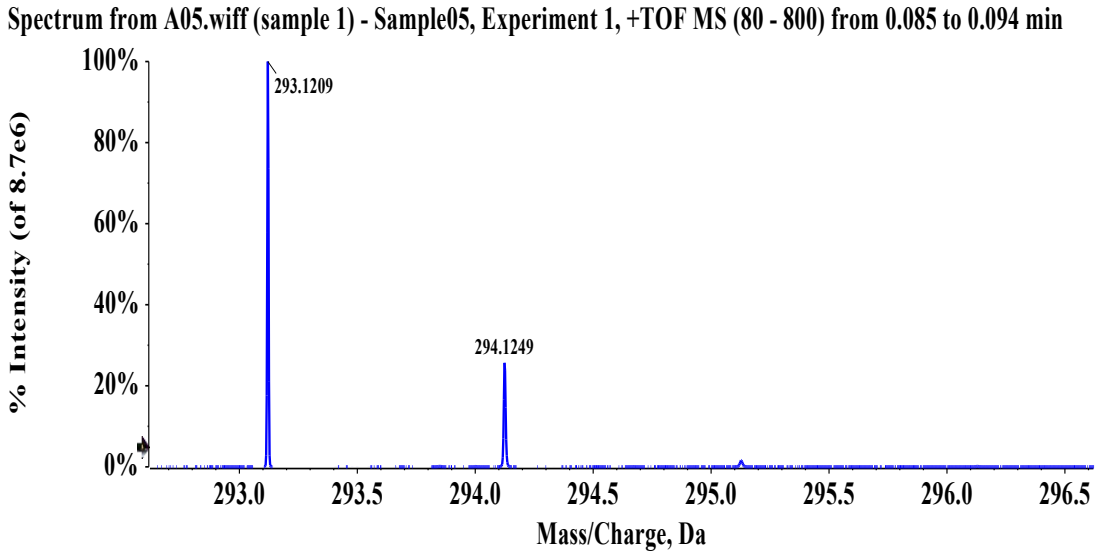

Figure 18. HRMS sprectrum of title compound 5e

Compound 5f

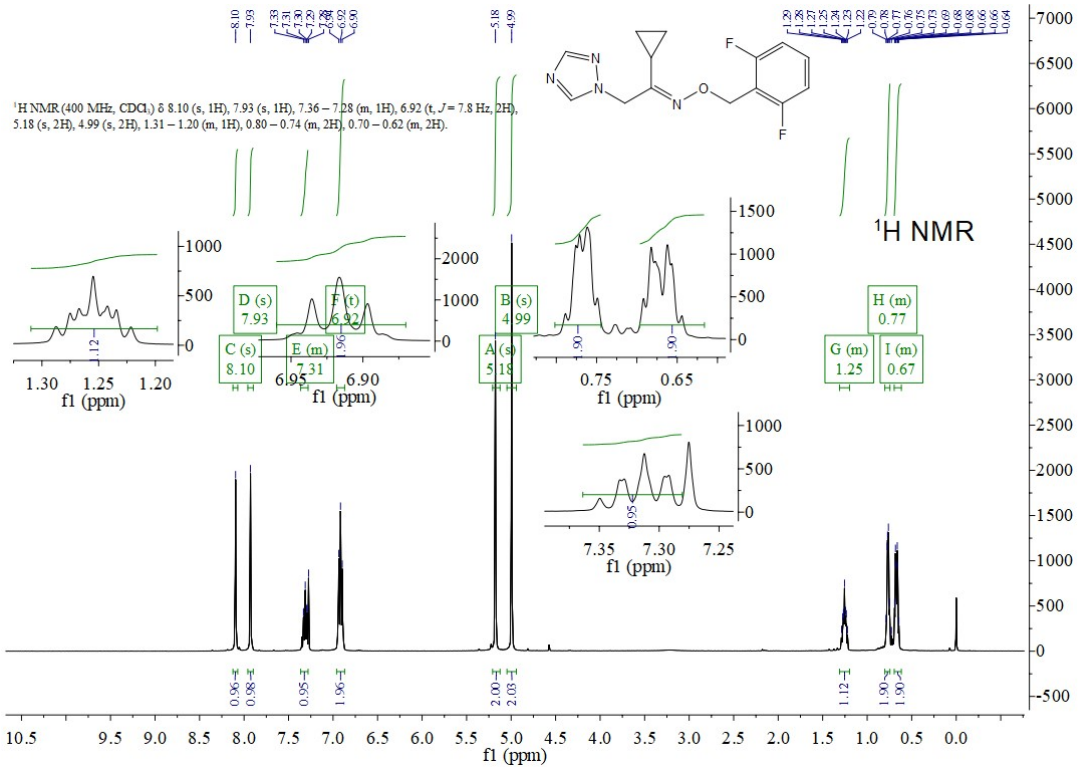

Figure 19. ^{1}H NMR sprectrum of intermediate 5f

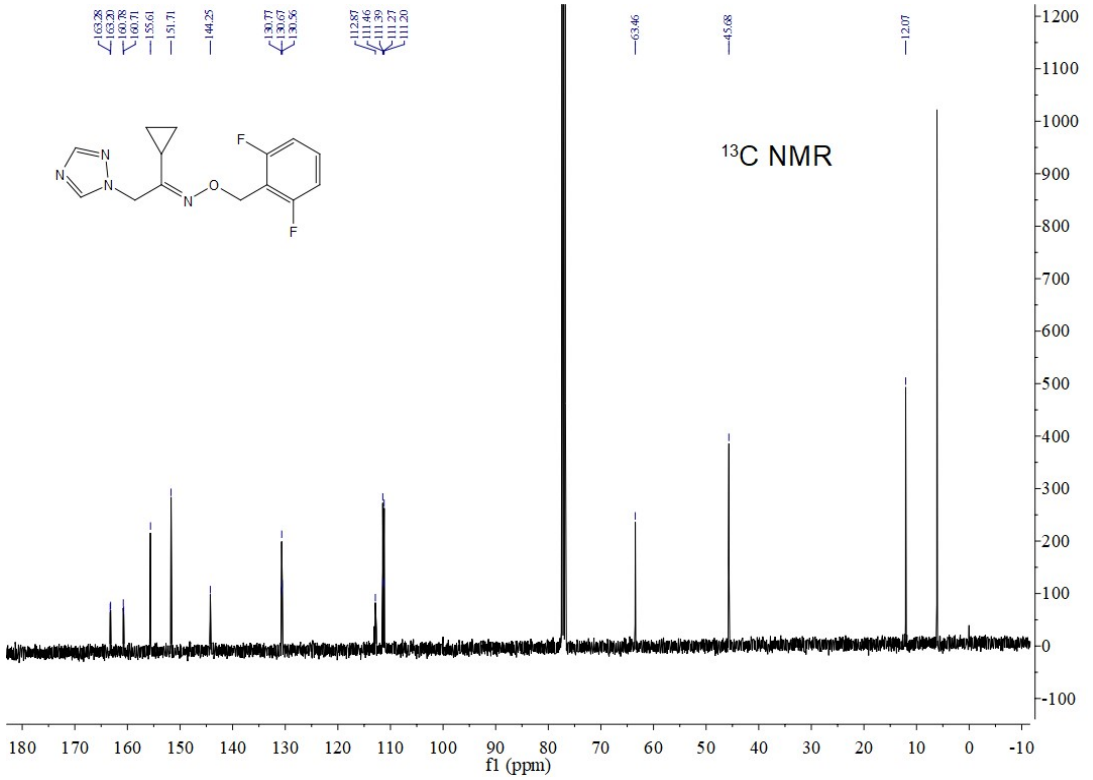

Figure 20. ^{13}C NMR sprectrum of title compound 5f

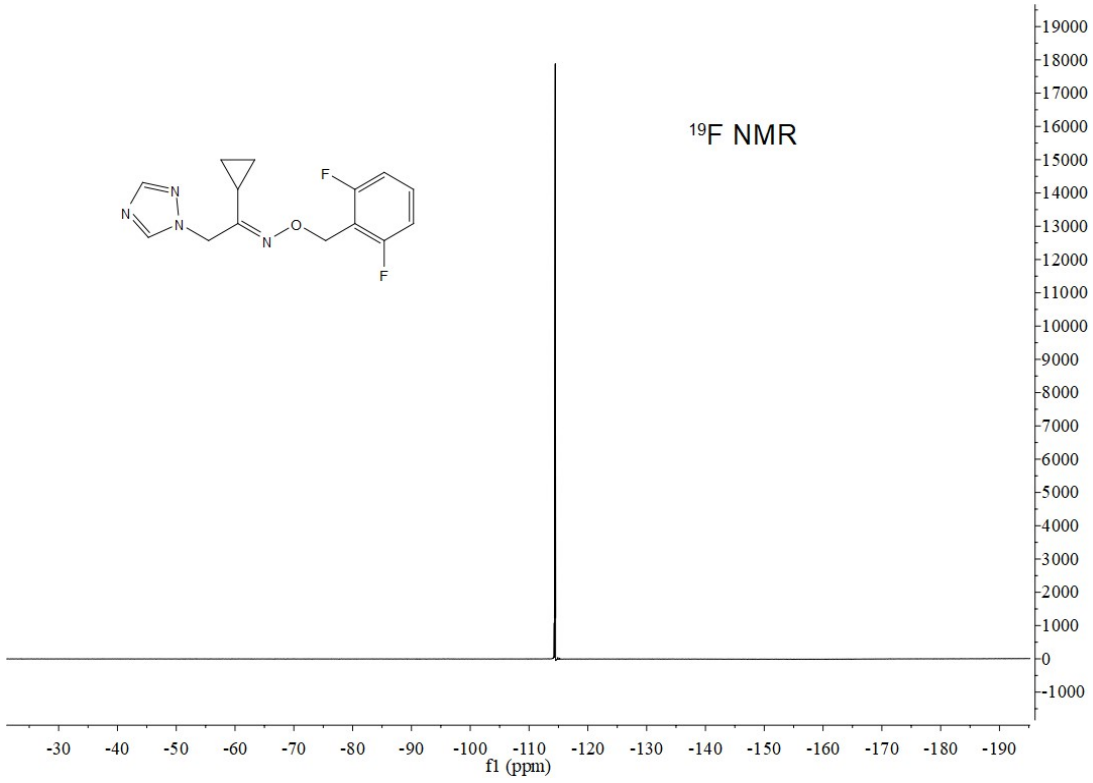

Figure 21. ^{19}F NMR sprectrum of title compound 5f

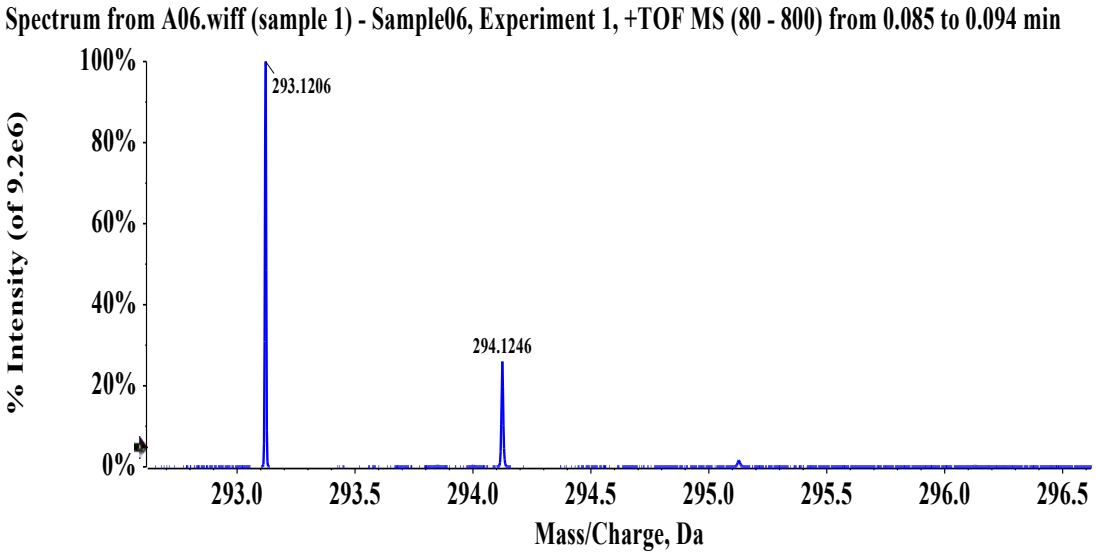

Figure 22. HRMS sprectrum of title compound 5f

Compound 5g

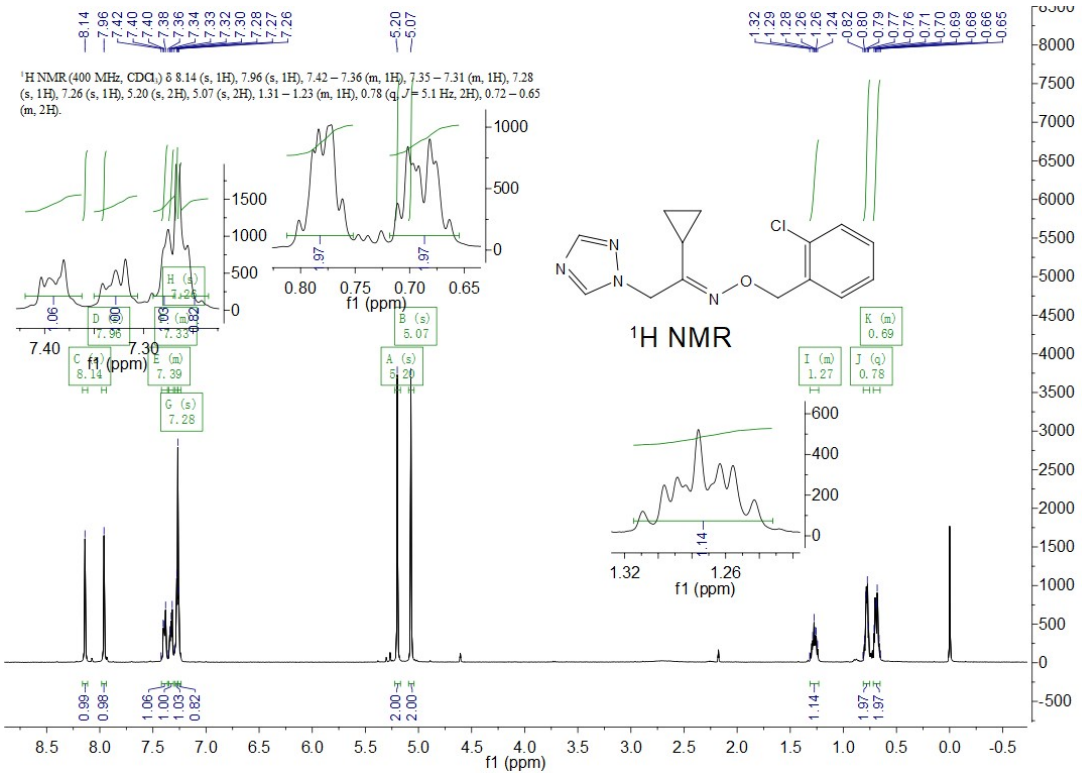

Figure 23. ^{1}H NMR sprectrum of title compound 5g

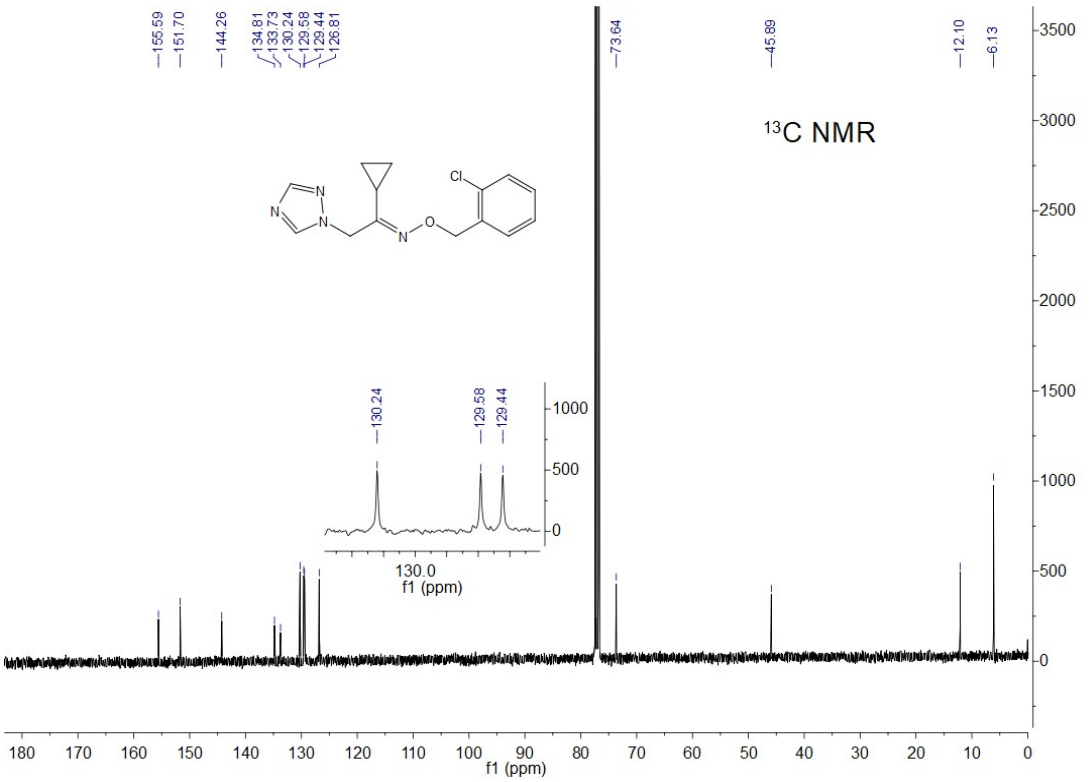

Figure24. ^{13}C NMR sprectrum of title compound 5g

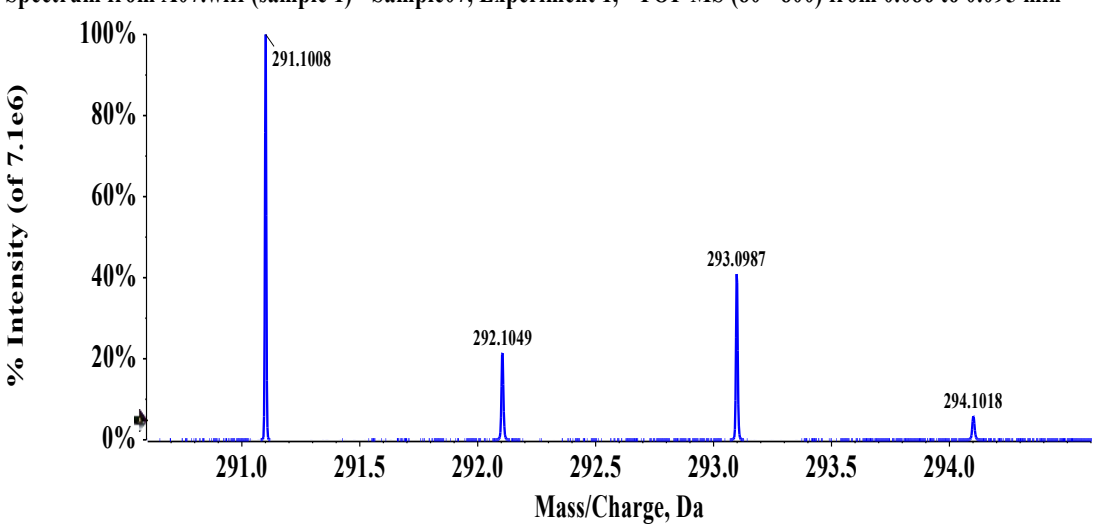

Figure 25. HRMS sprectrum of title compound 5g

Compound 5h

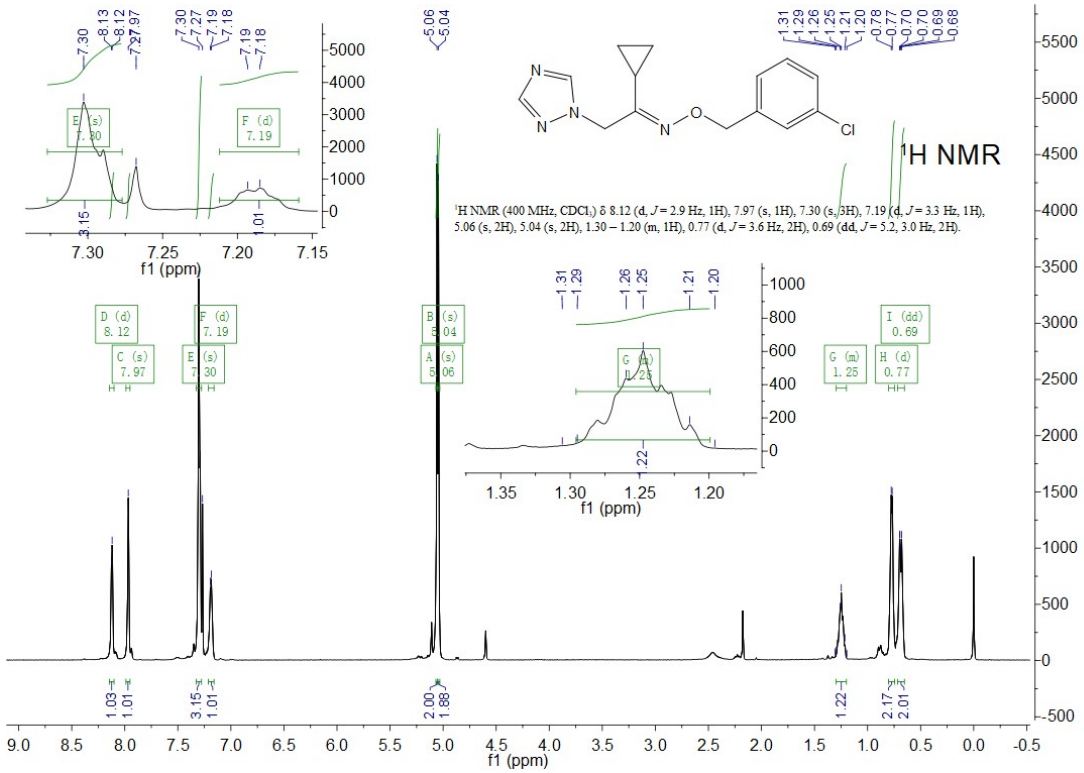

Figure 26. ^{1}H NMR sprectrum of title compound 5h

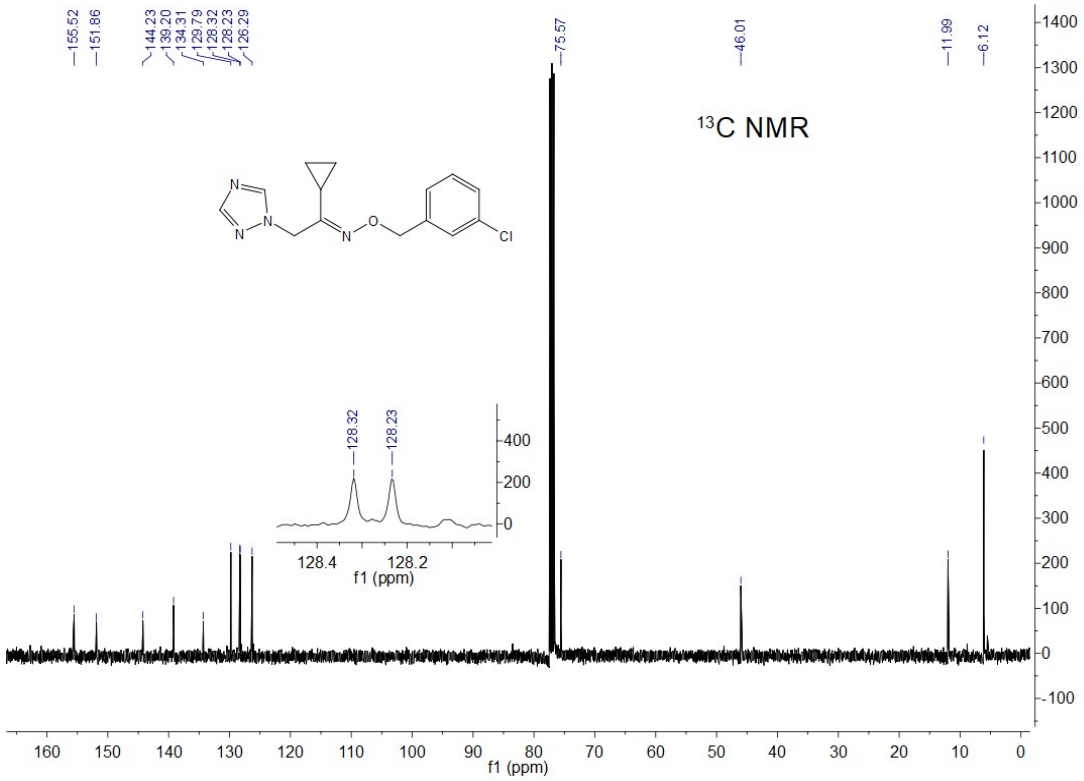

Figure 27. ^{13}C NMR sprectrum of title compound 5h

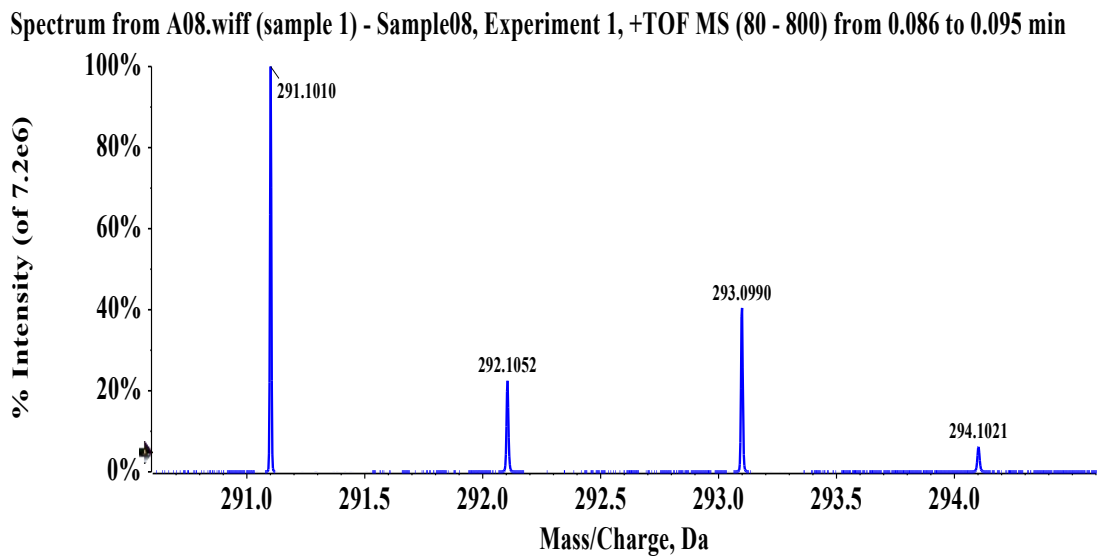

Figure 28. HRMS sprectrum of title compound 5h

Compound 5i

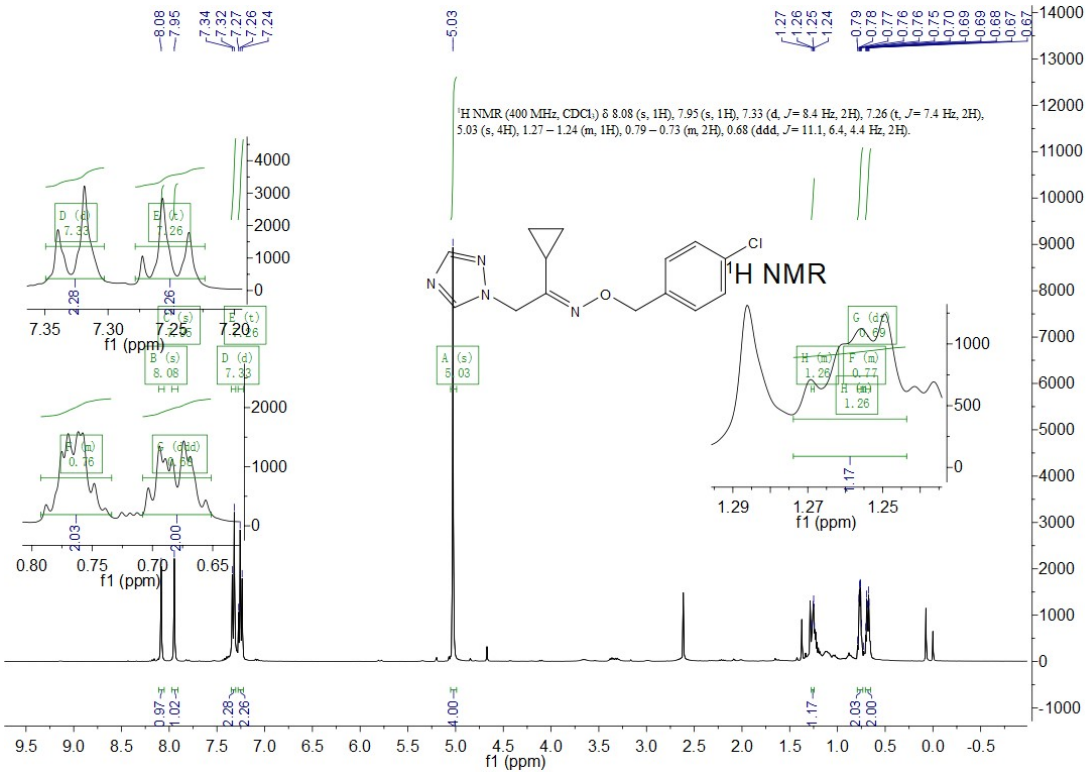

Figure 29. ^{1}H NMR sprectrum of title compound 5i

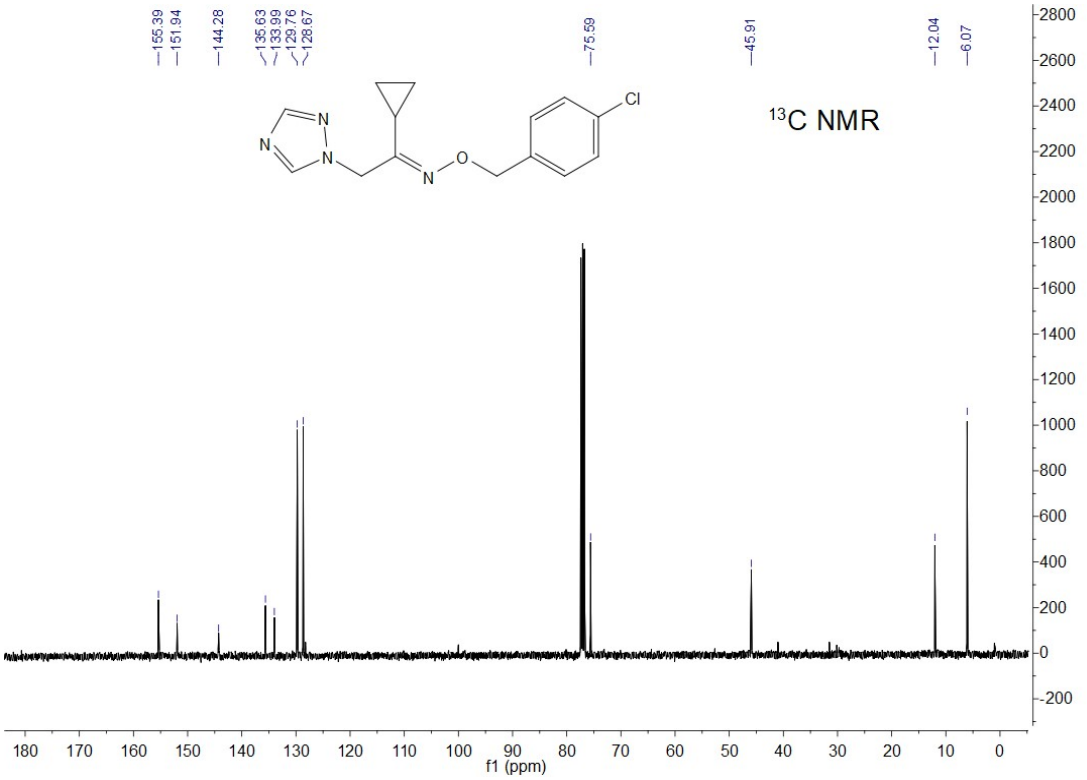

Figure 30. ^{13}C NMR sprectrum of title compound 5i

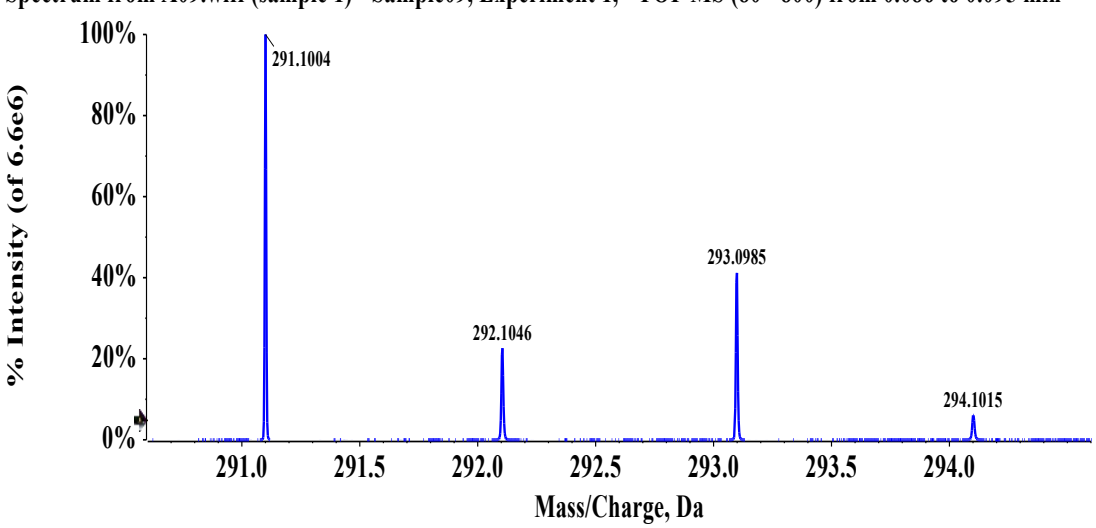

Figure 31. HRMS sprectrum of title compound 5i

Compound 5j

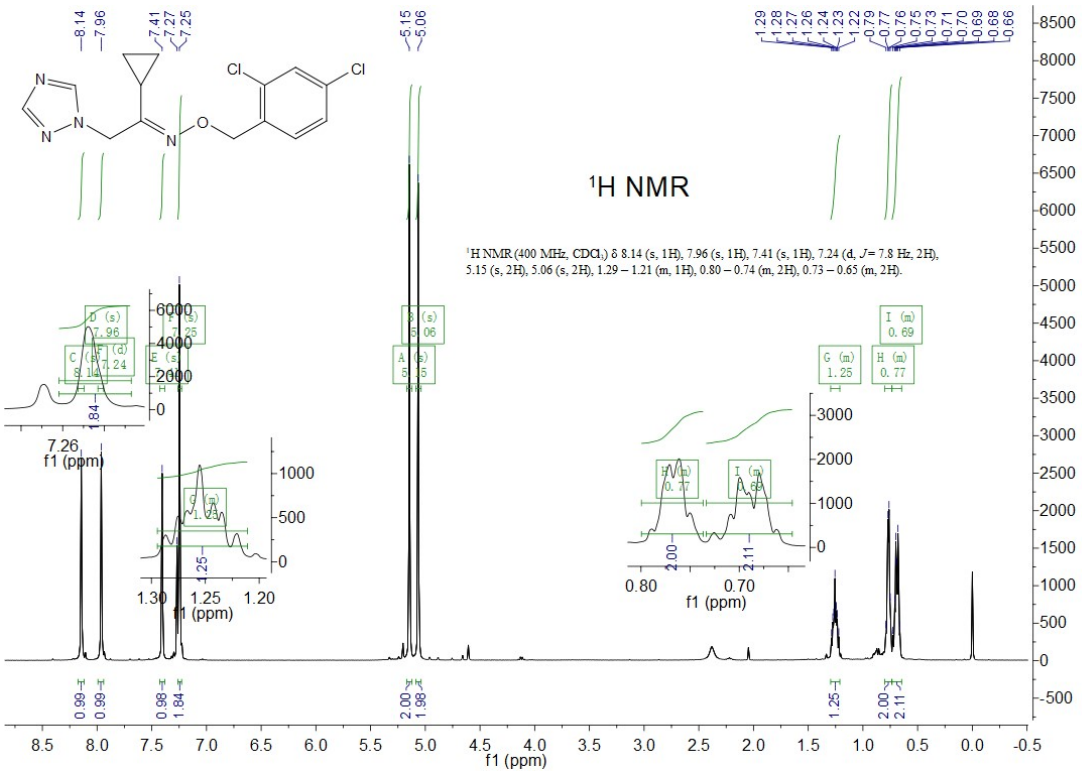

Figure 32. ^{1}H NMR sprectrum of title compound 5j

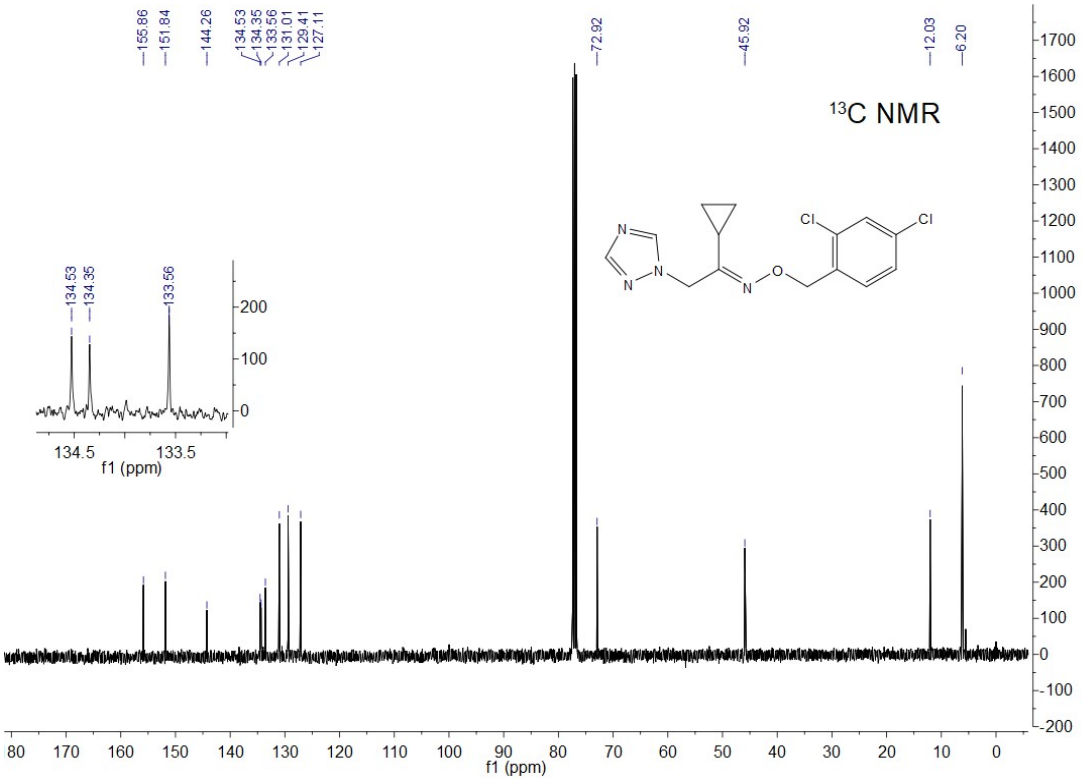

Figure 33. ^{13}C NMR sprectrum of title compound 5j

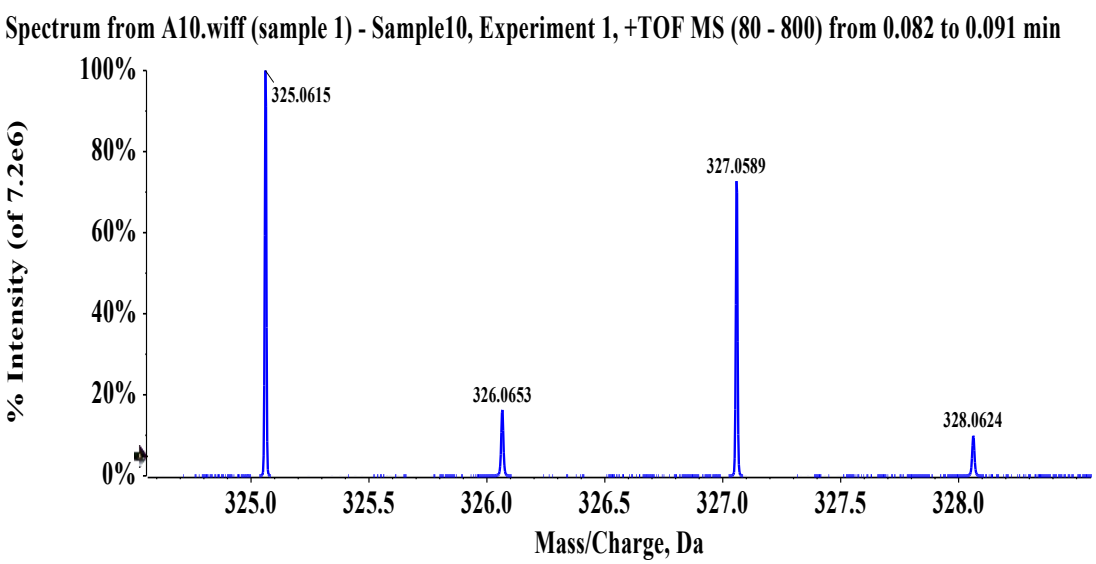

Figure 34. HRMS sprectrum of title compound 5j

Compound 5k

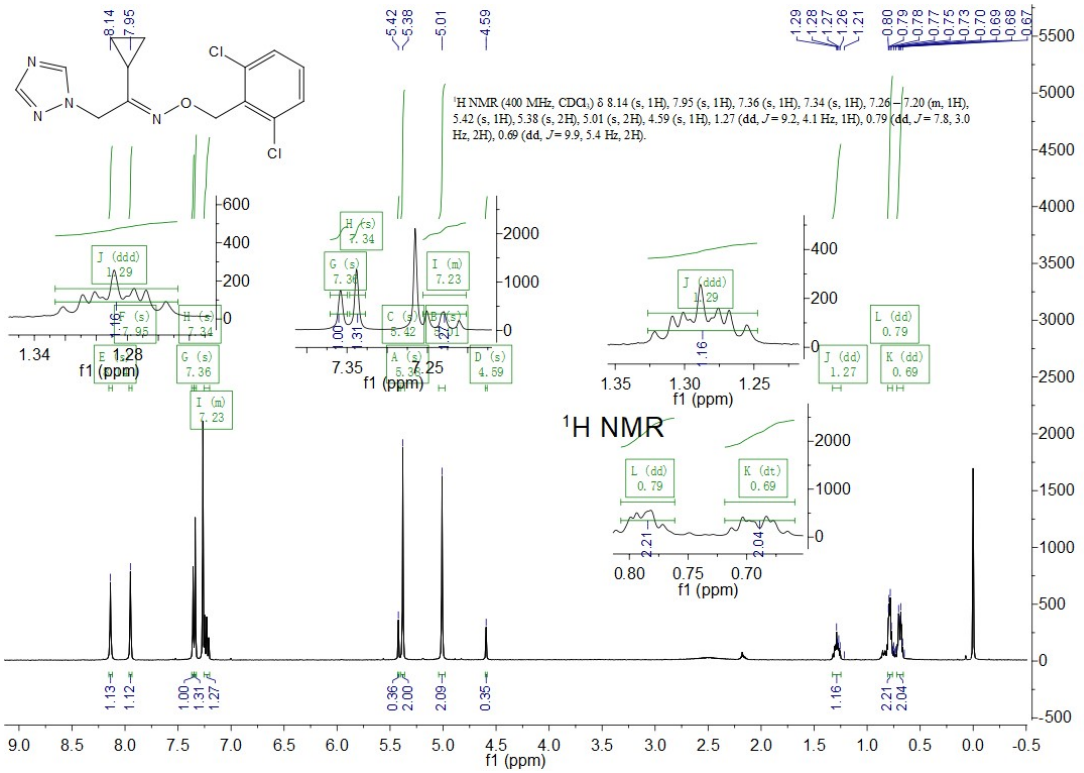

Figure 35. ^{1}H NMR spectrum of title compounde 5k

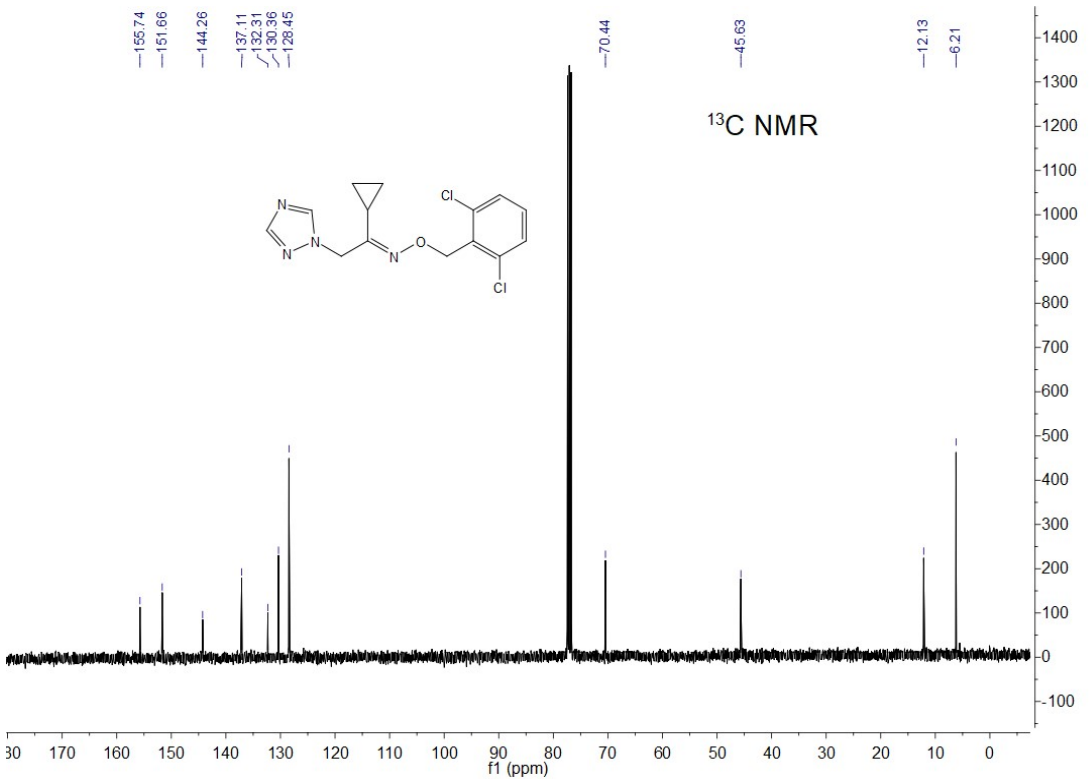

Figure 36.^{13}C NMR sprectrum of title compound 5k

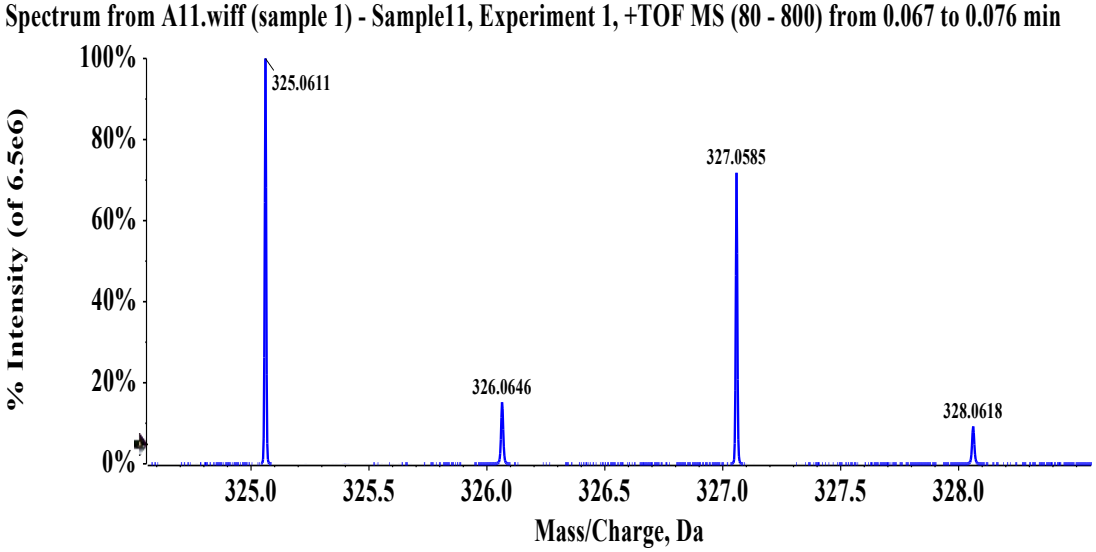

Figure 37. HRMS sprectrum of title compound 5k

Compound 5l

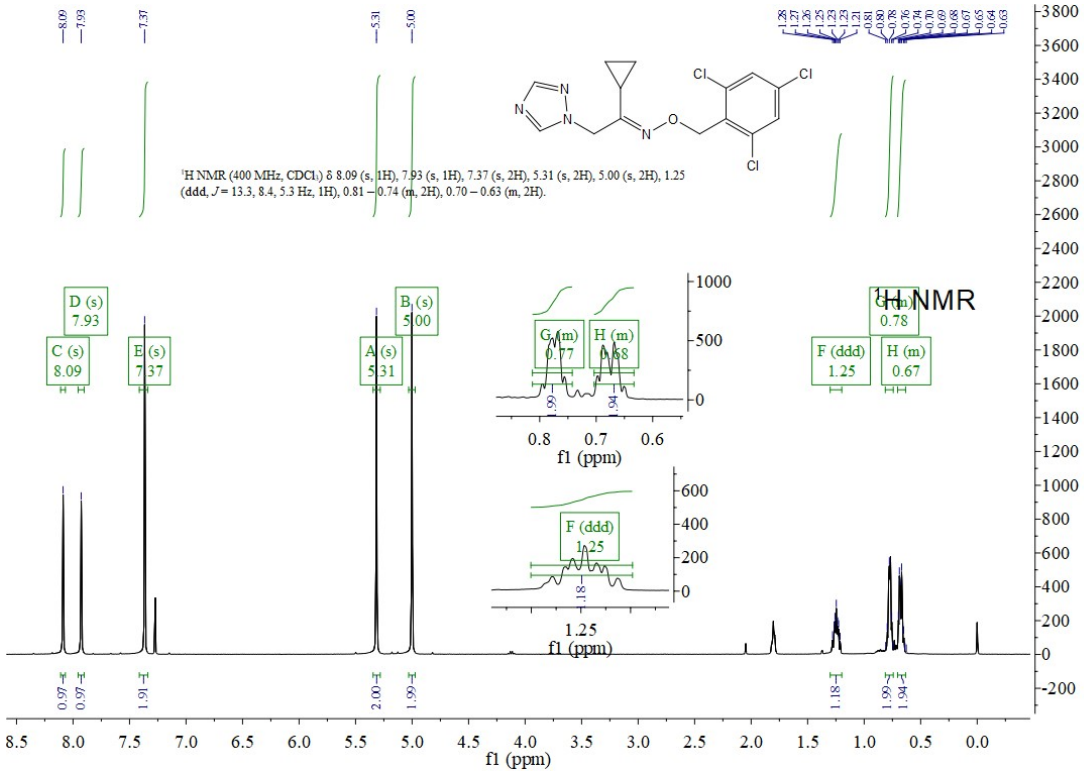

Figure 38. ^{1}H NMR sprectrum of title compound 5l

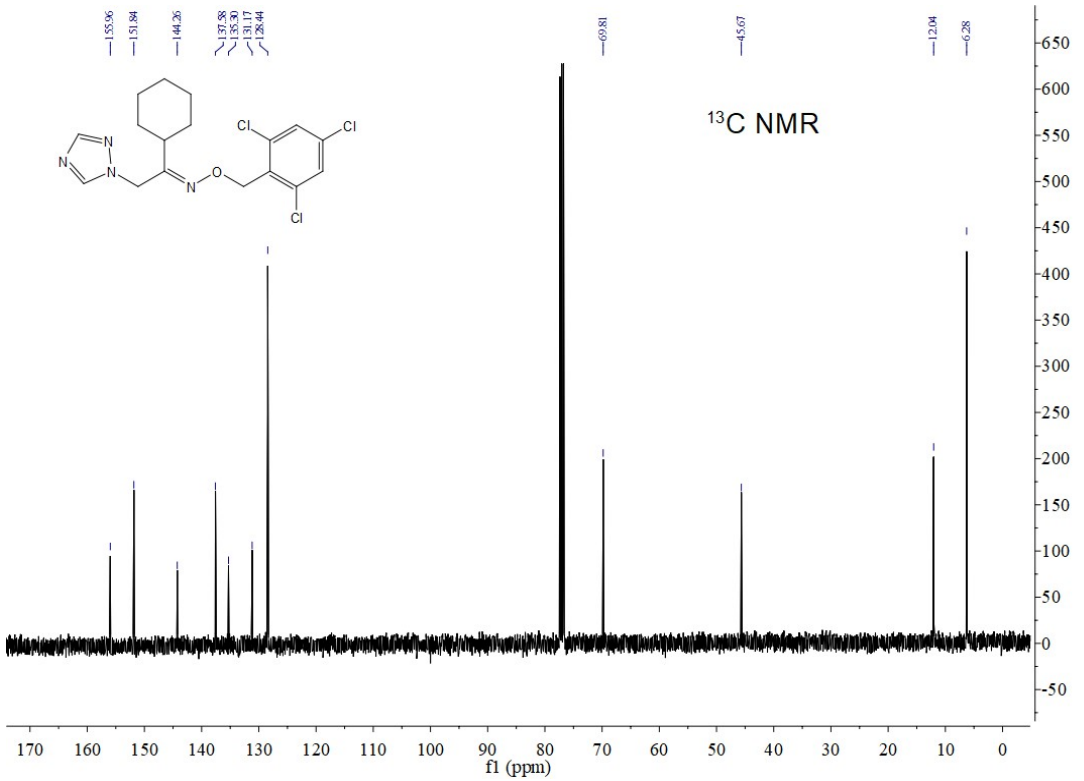

Figure 39. ^{13}C NMR sprectrum of title compound 5l

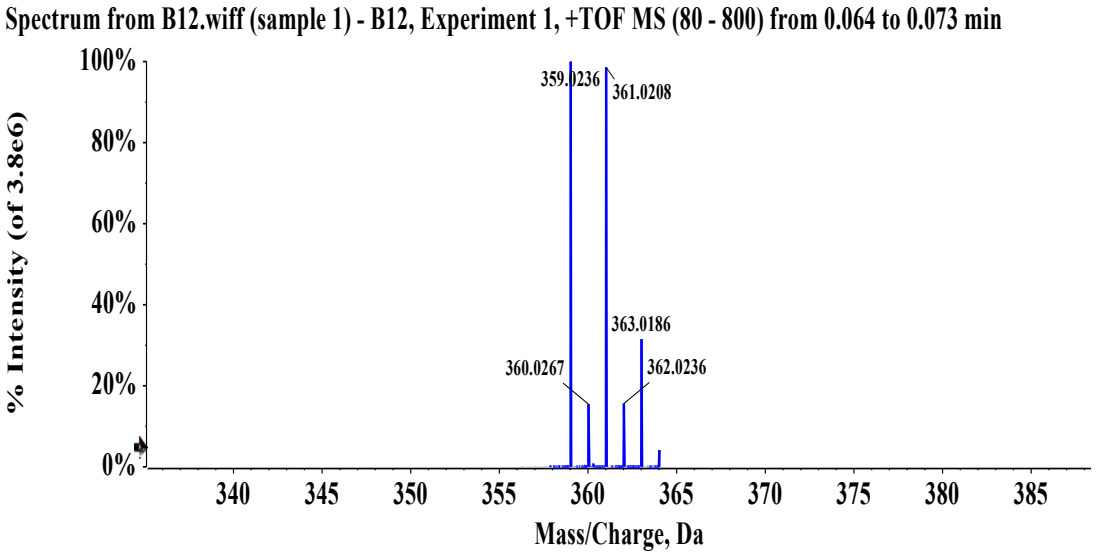

Figure 40. HRMS sprectrum of title compound 5l

Compound 5m

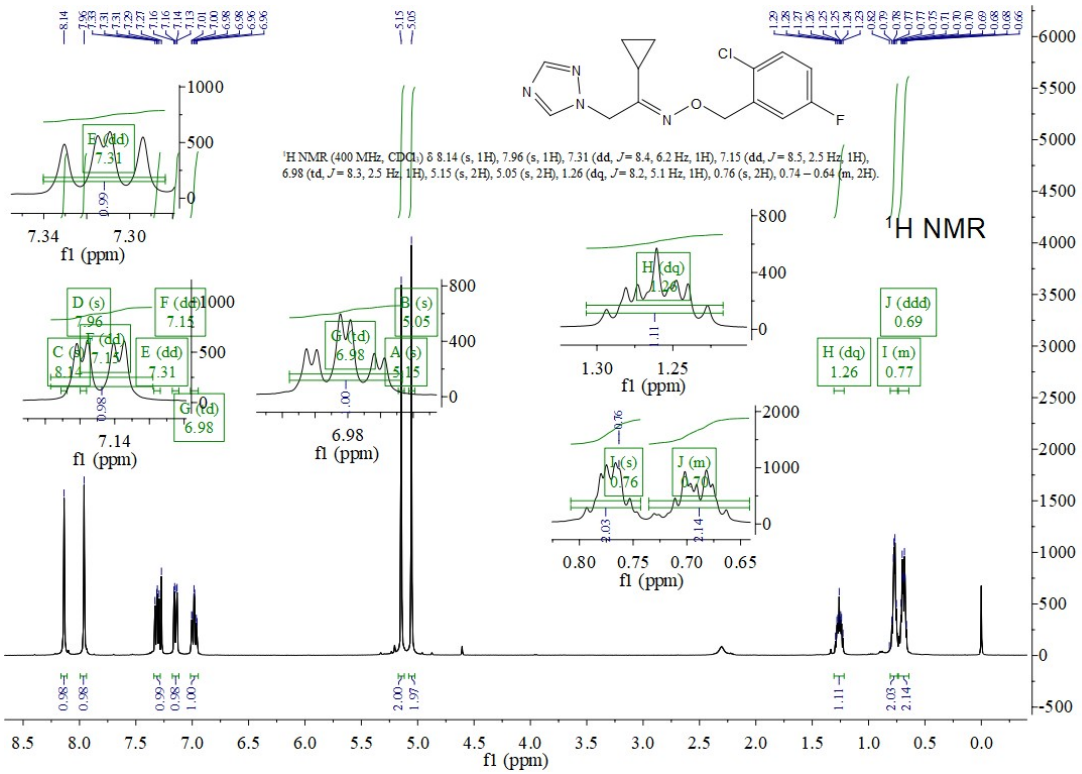

Figure 41.^{1}H NMR sprectrum of title compound 5m

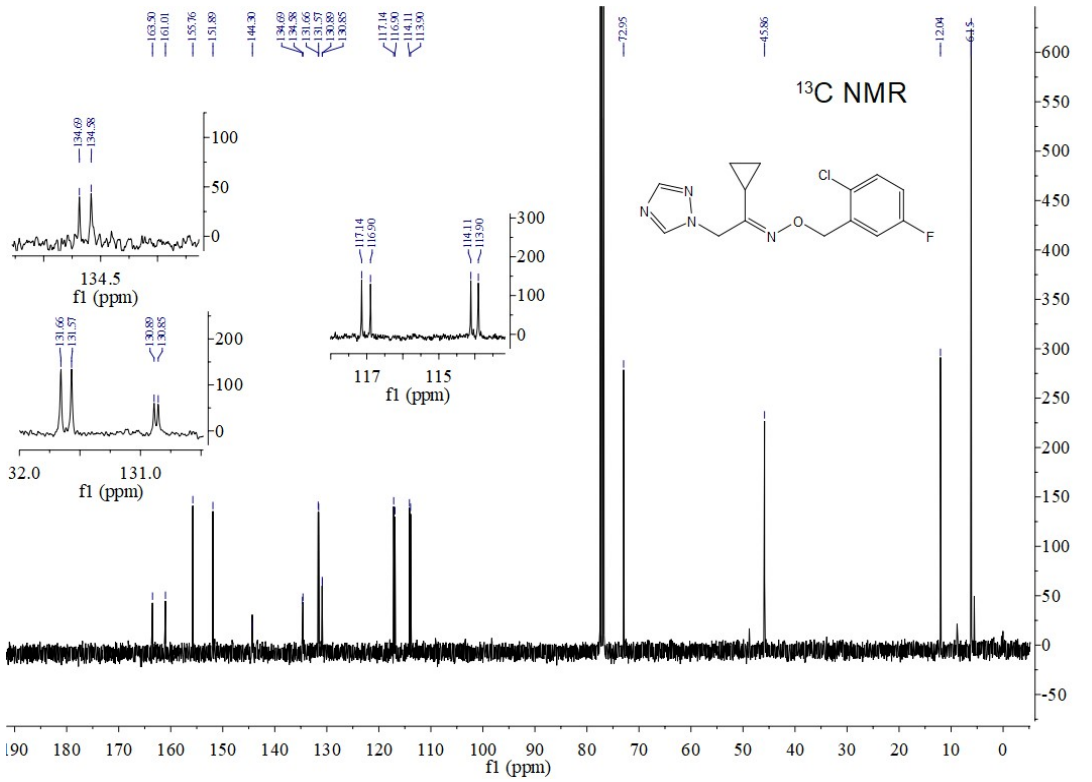

Figure 42.^{13}C NMR sprectrum of title compound 5m

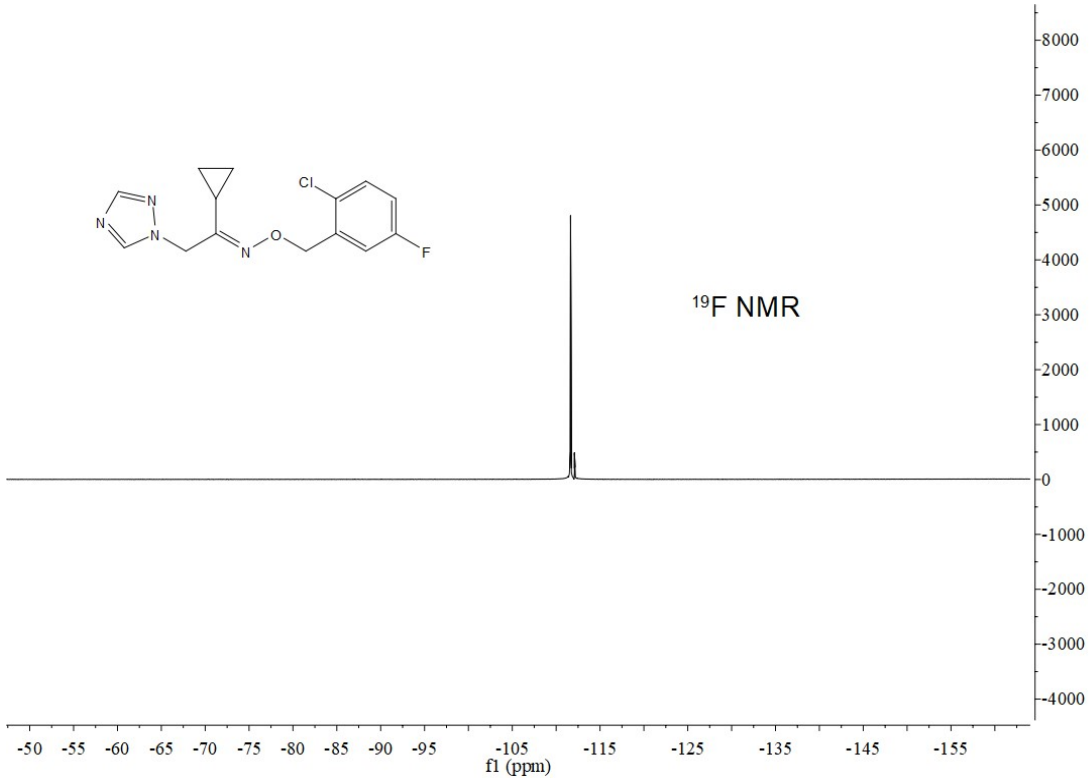

Figure 43. ^{19}F NMR sprectrum of title compound 5m

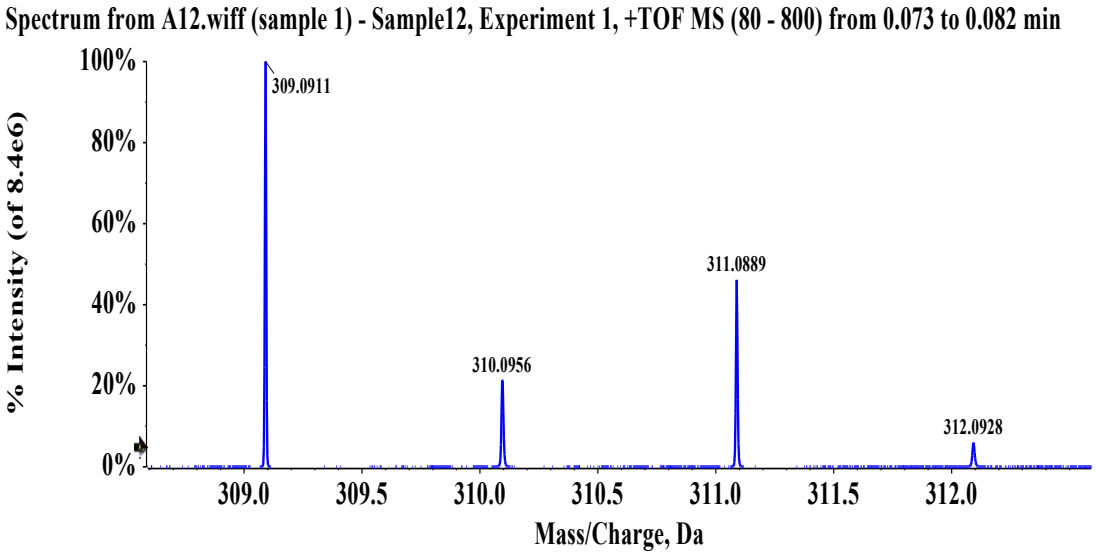

Figure 44. HRMS sprectrum of title compound 5m

Compound 5n

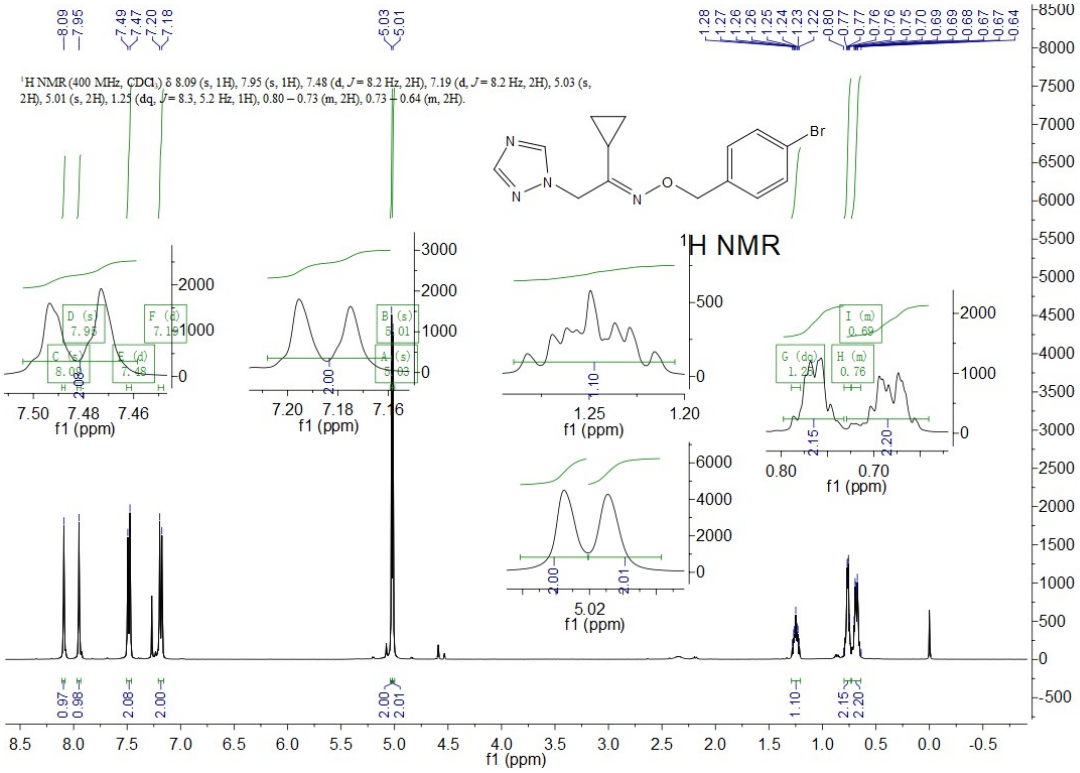

Figure 45.^{1}H NMR sprectrum of title compound 5n

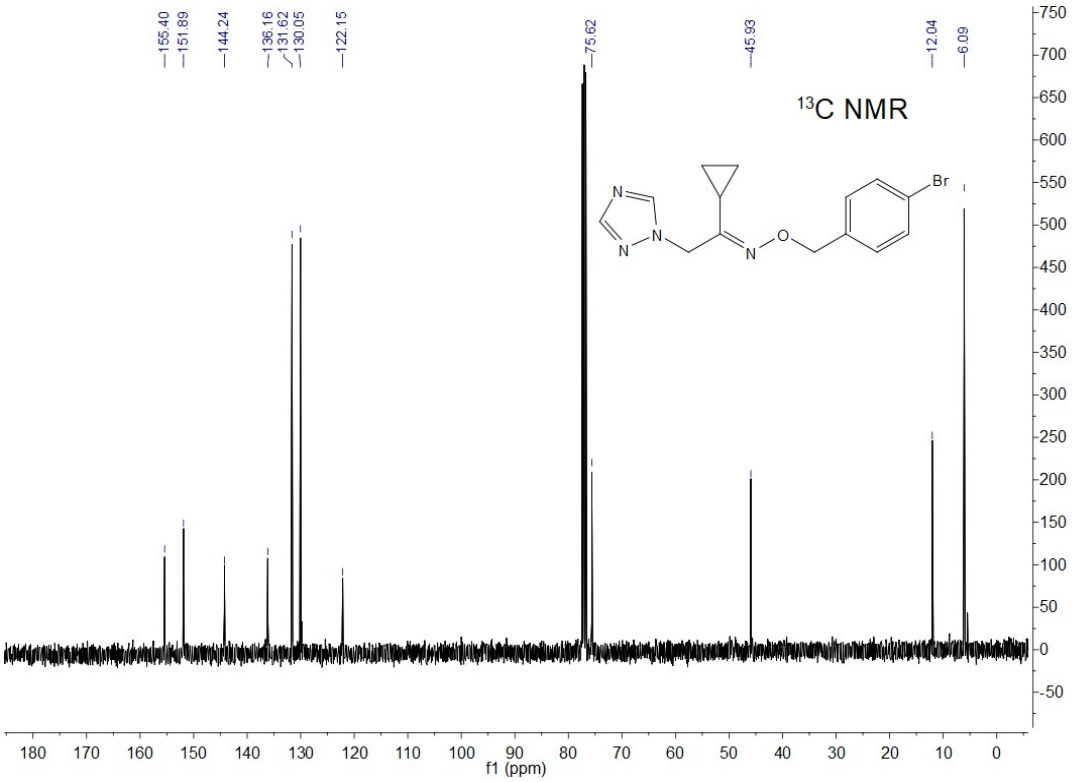

Figure46.^{13}C NMR sprectrum of title compound 5n

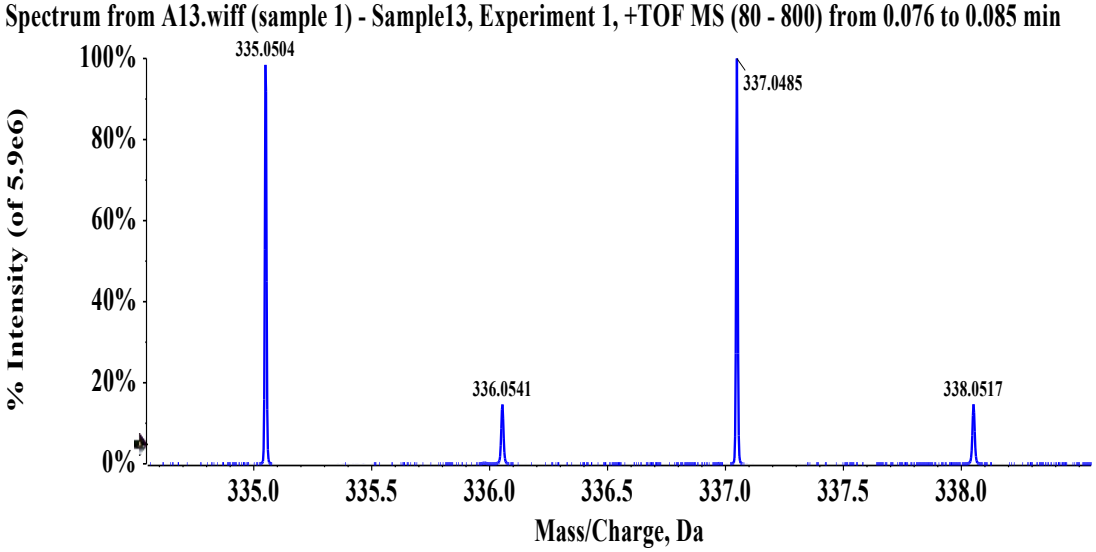

Figure 47. HRMS sprectrum of title compound 5n

Compound 5o

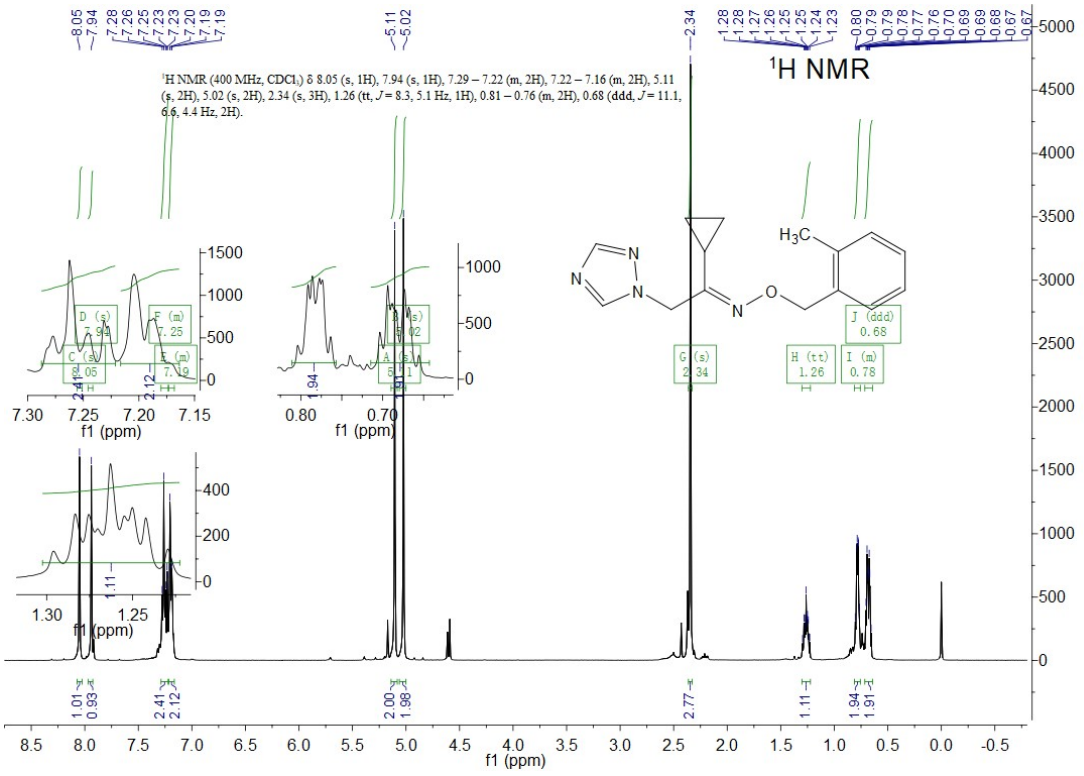

Figure 48. ^{1}H NMR sprectrum of title compound 5o

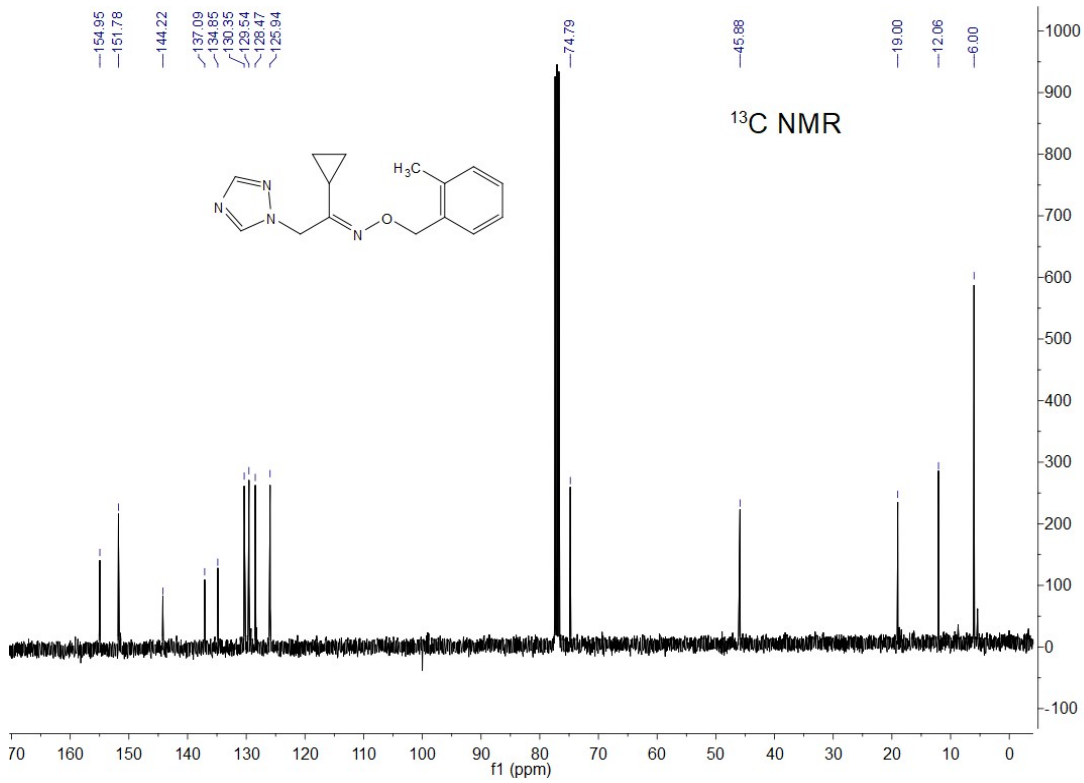

Figure 49. ^{13}C NMR sprectrum of title compound 5o

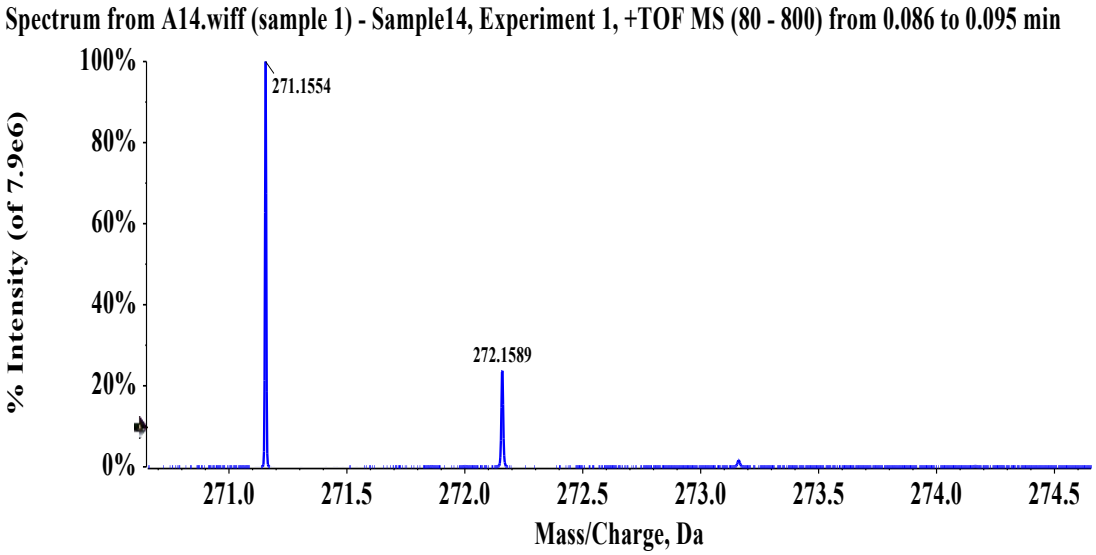

Figure 50. HRMS sprectrum of title compound 5o

Compound 5p

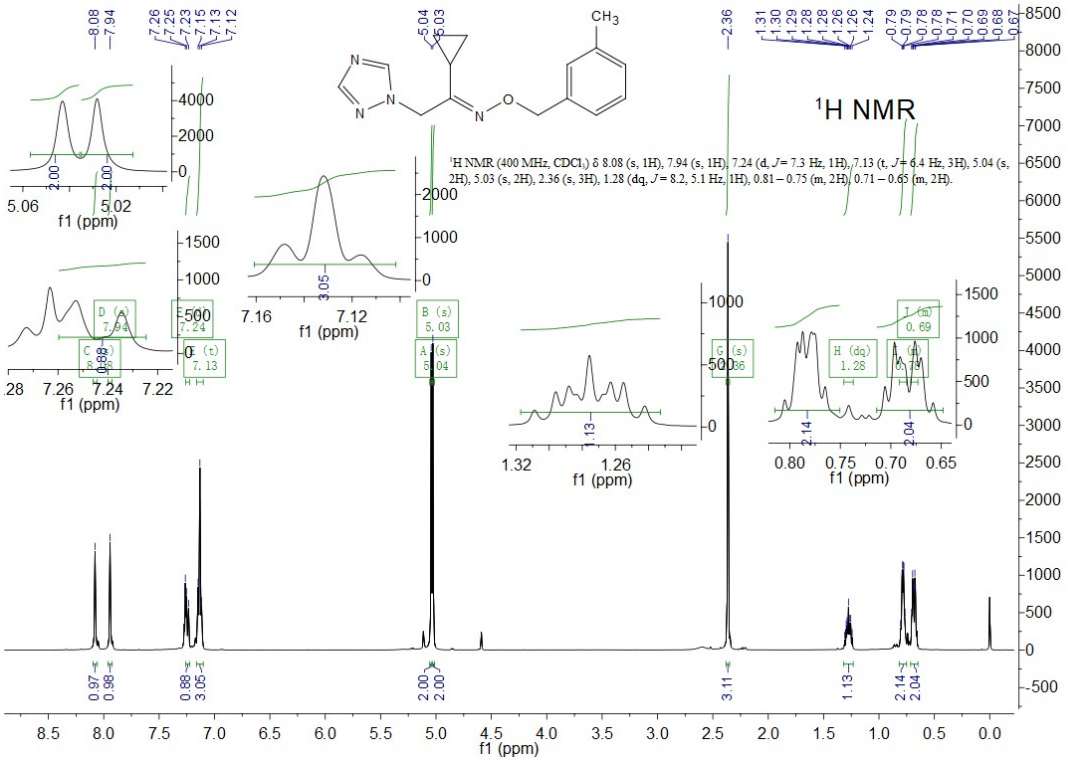

Figure 51. ^{1}H NMR sprectrum of title compound 5p

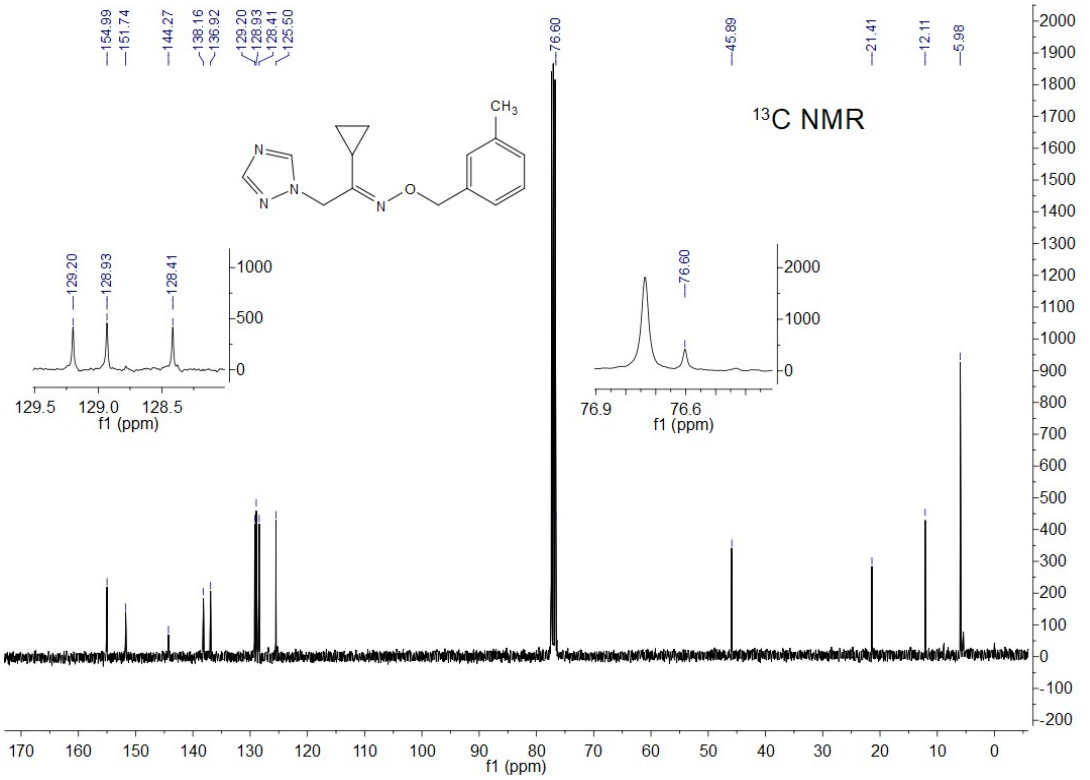

Figure 52. ^{13}C NMR sprectrum of title compound 5p

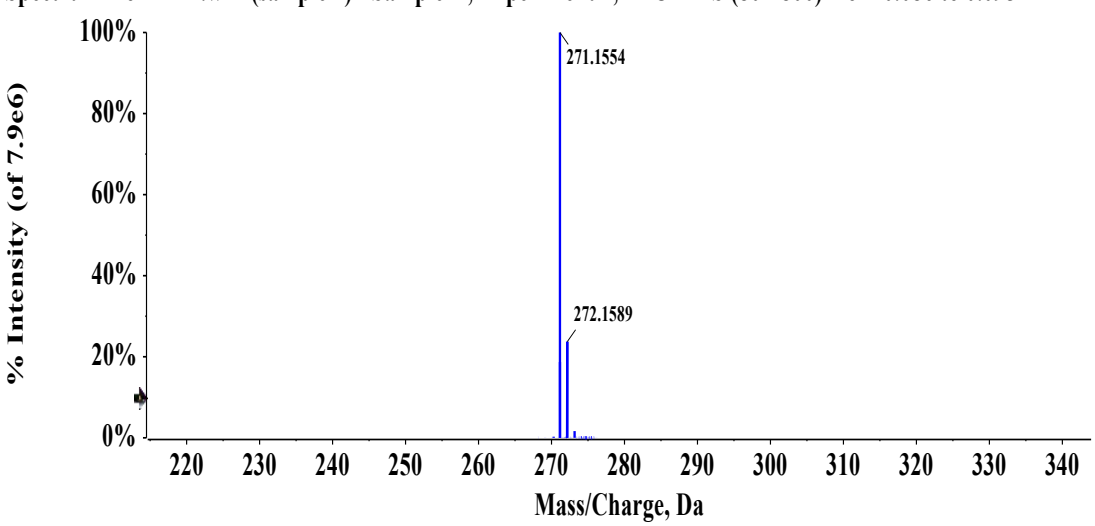

Figure 53. HRMS sprectrum of title compound 5p

Compound 5q

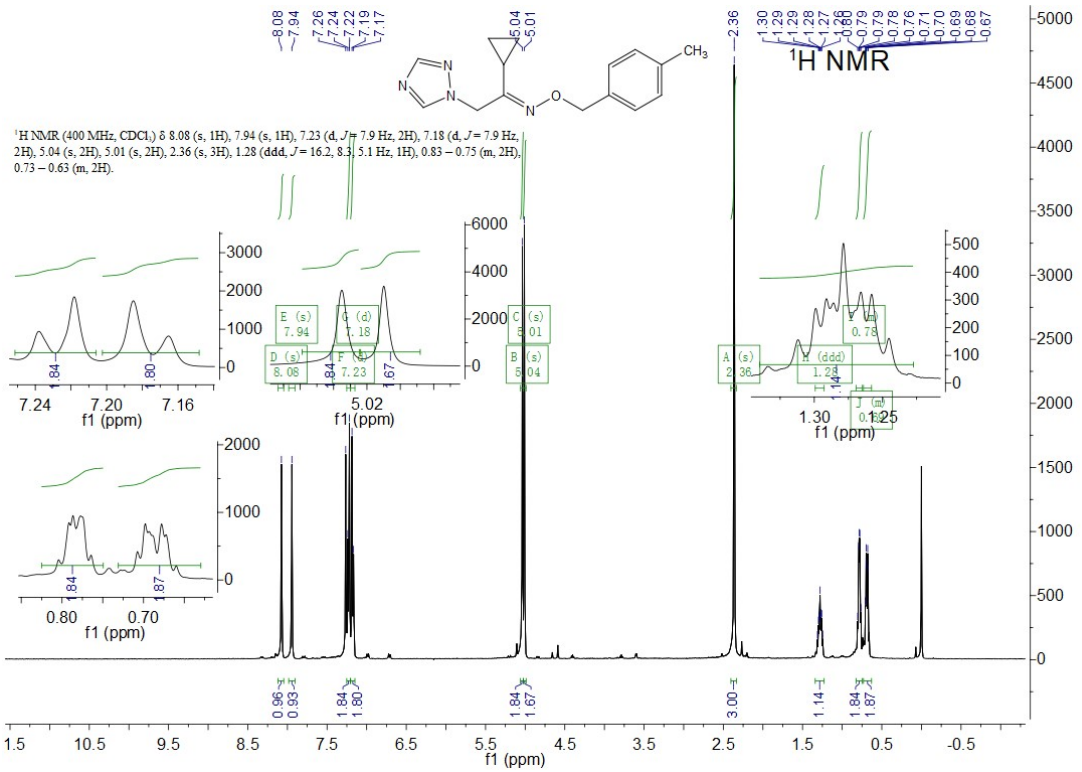

Figure 54. ^{1}H NMR sprectrum of title compound 5q

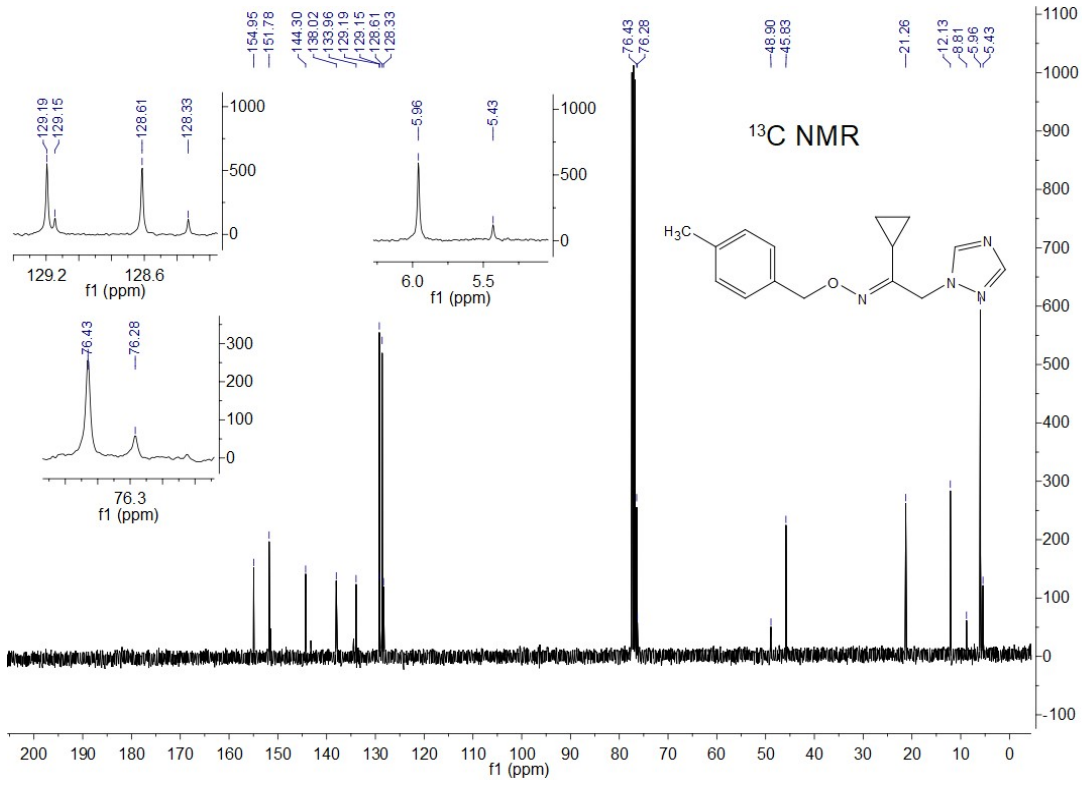

Figure 55. ^{13}C NMR sprectrum of title compound 5q

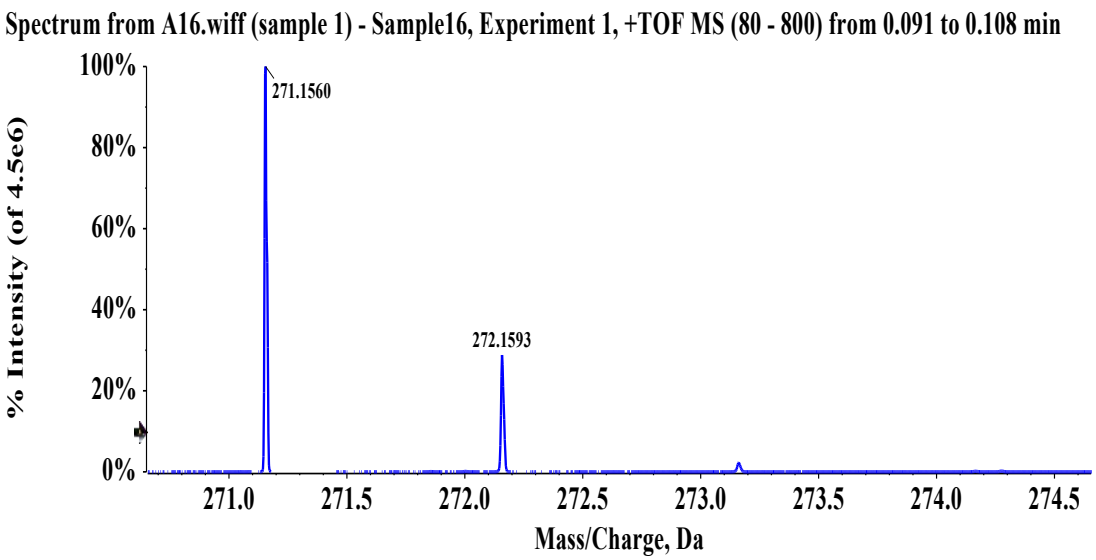

Figure 56. HRMS sprectrum of title compound 5q

Compound 5r

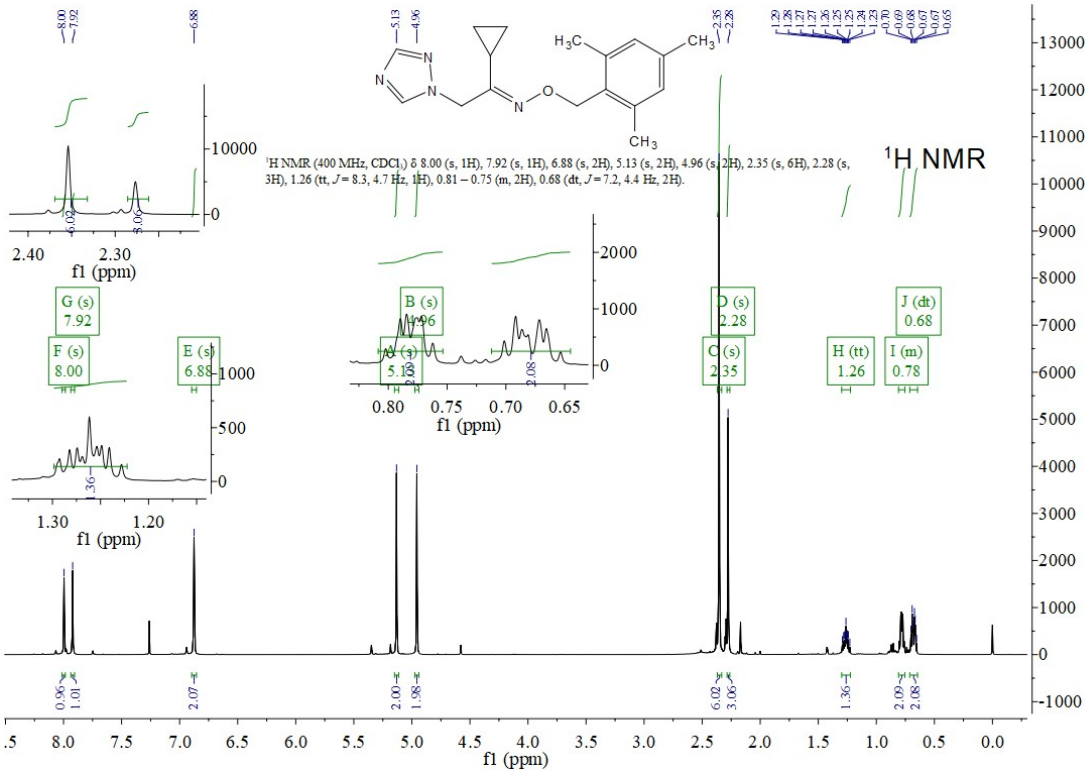

Figure 57. ^{1}H NMR sprectrum of title compound 5r

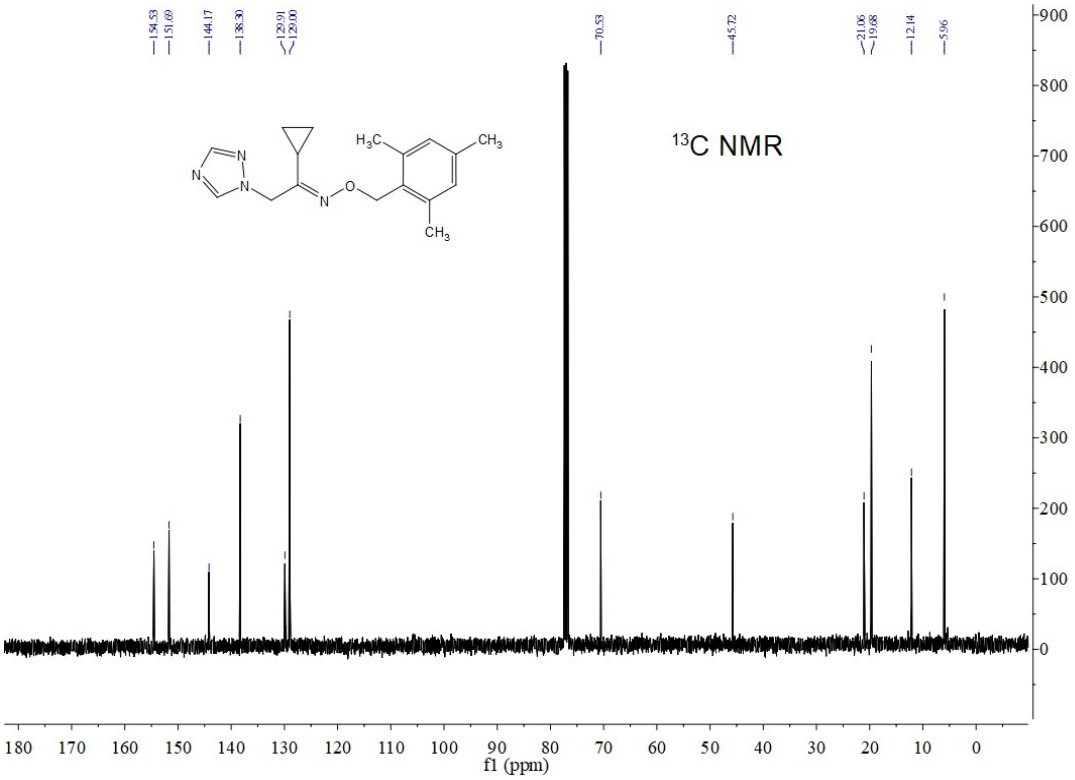

Figure 58. ^{13}C NMR sprectrum of title compound 5r

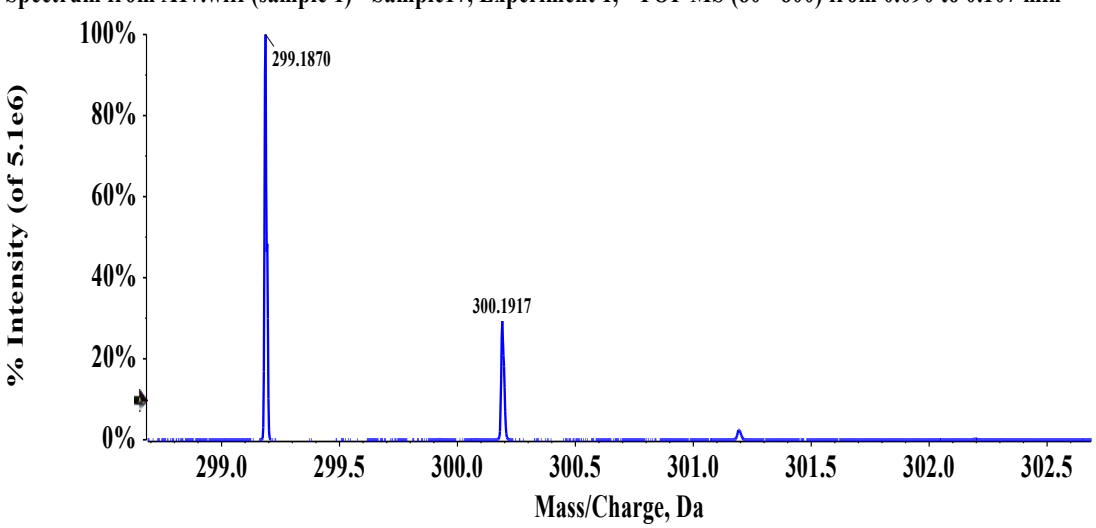

Figure 59. HRMS sprectrum of title compound 5r

Compound 5s

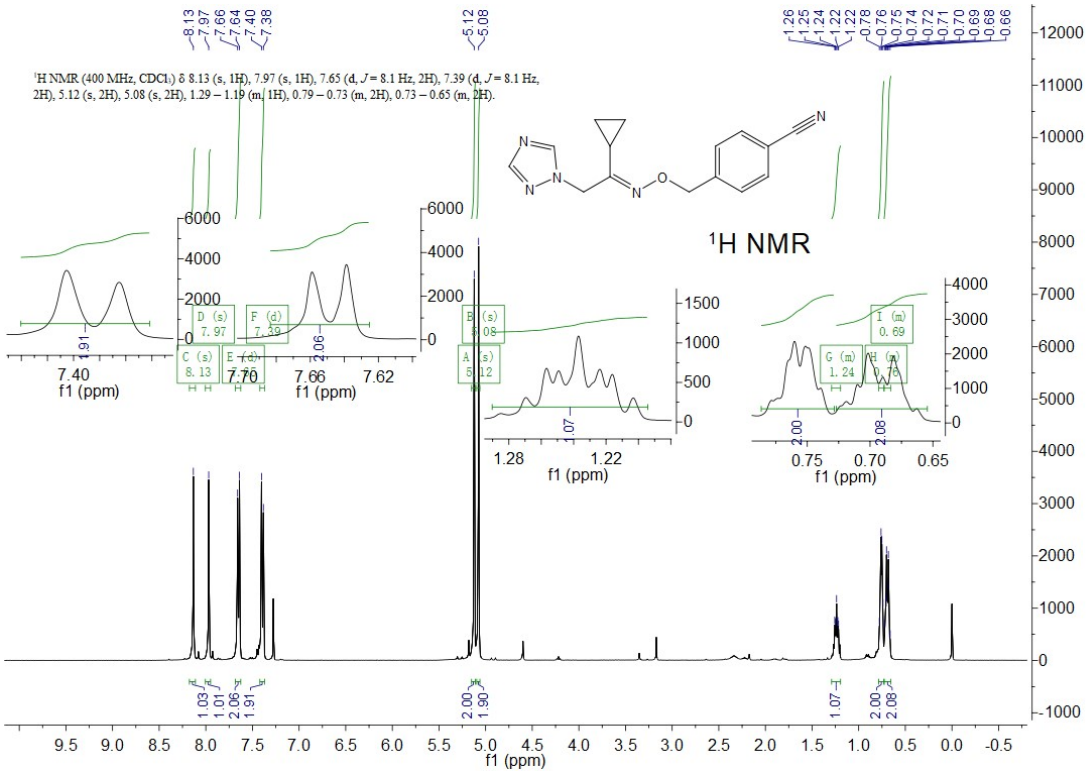

Figure 60. ^{1}H NMR sprectrum of title compound 5s

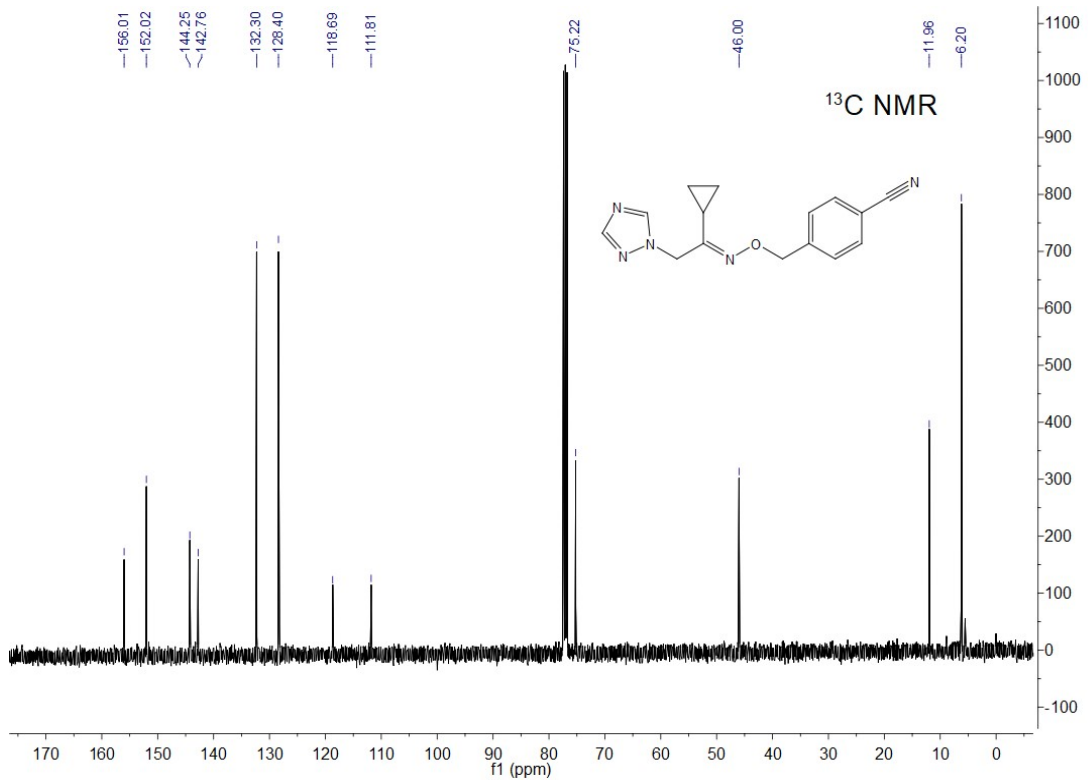

Figure 61. ^{13}C NMR sprectrum of title compound 5s

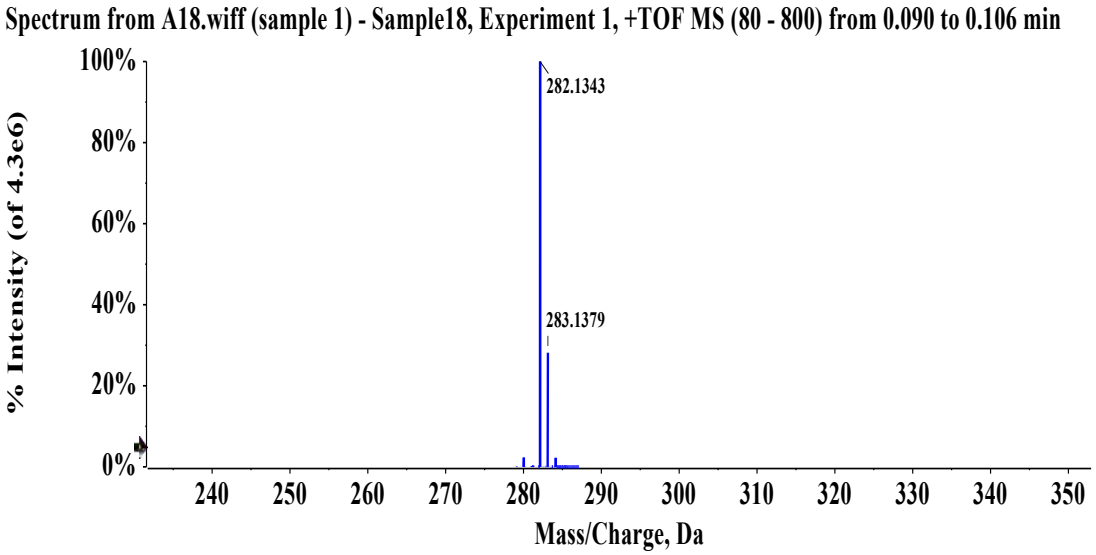

Figure 62. HRMS sprectrum of title compound 5s

Compound 5t

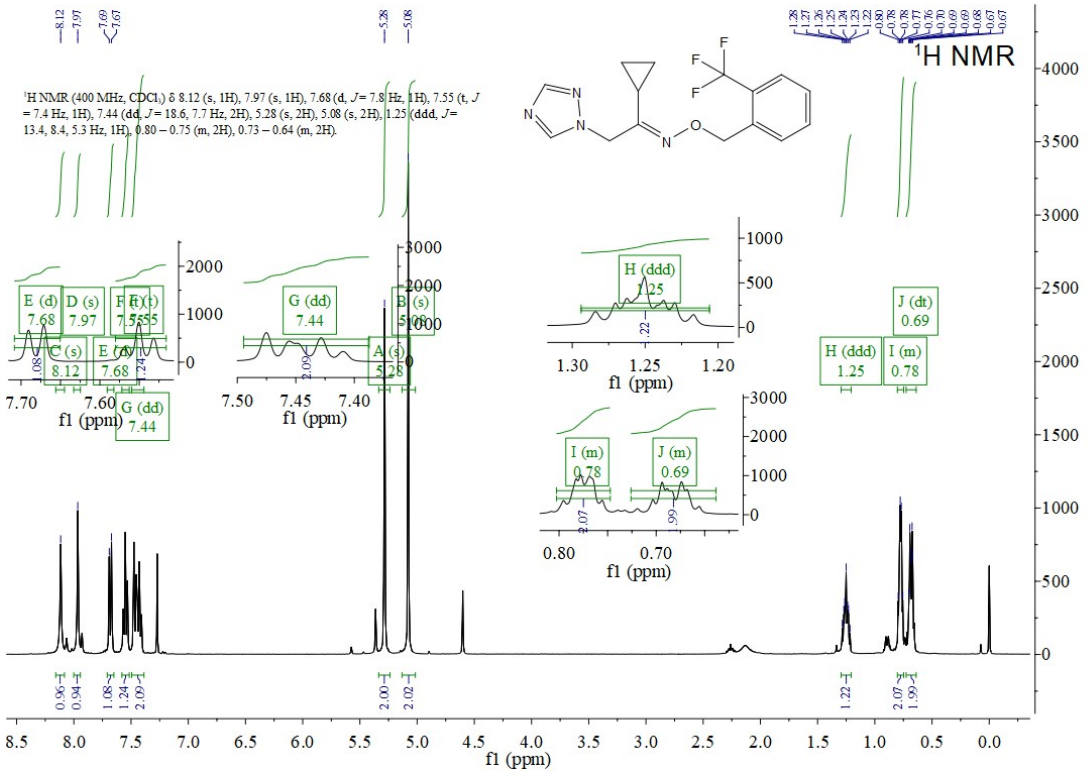

Figure 63. ^{1}H NMR sprectrum of title compound 5t

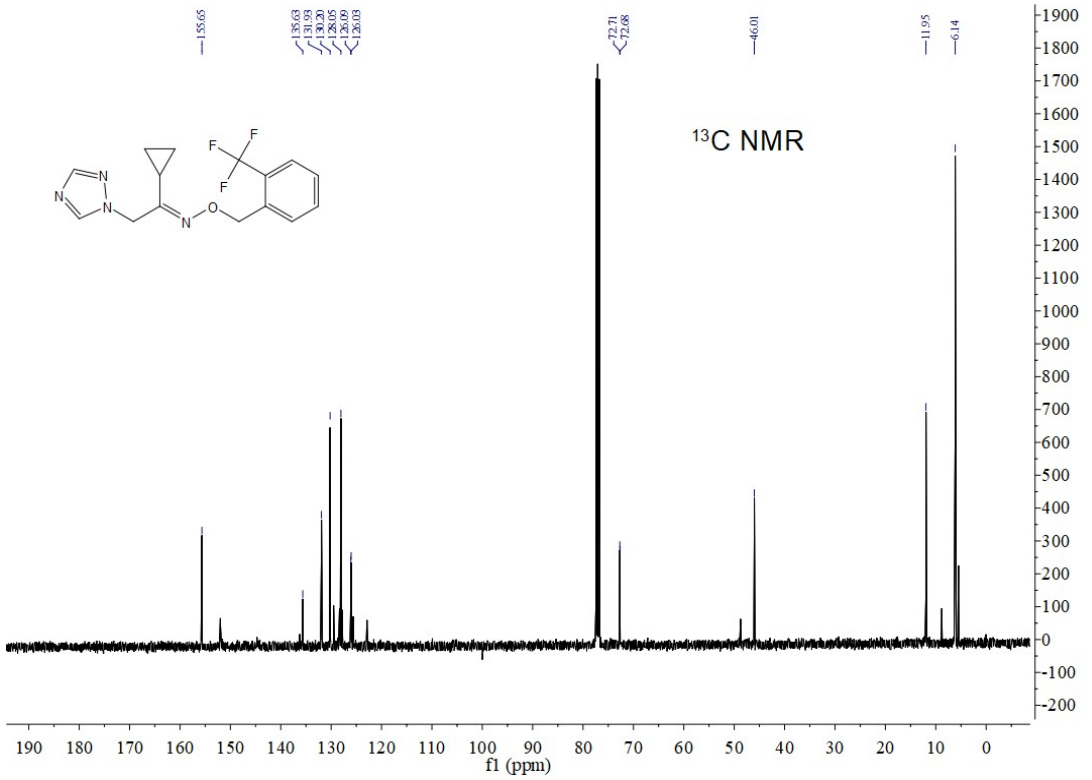

Figure 64. ^{13}C NMR sprectrum of title compound 5t

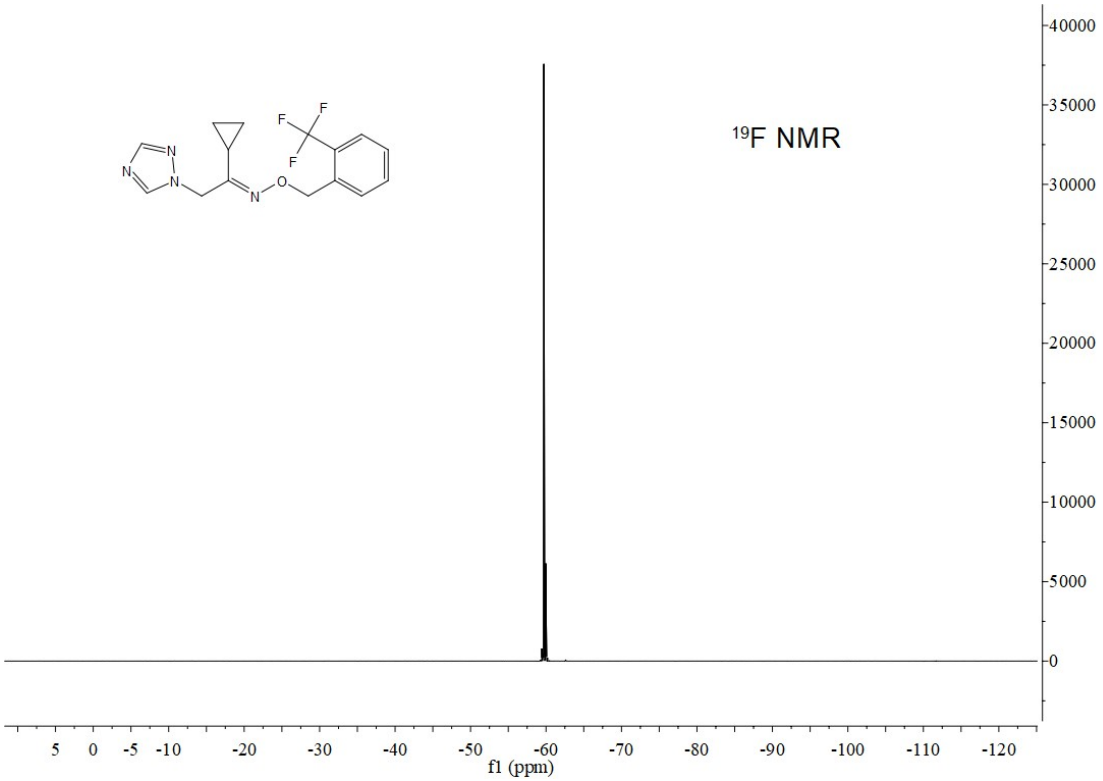

Figure 65. ^{19}F NMR sprectrum of title compound 5t

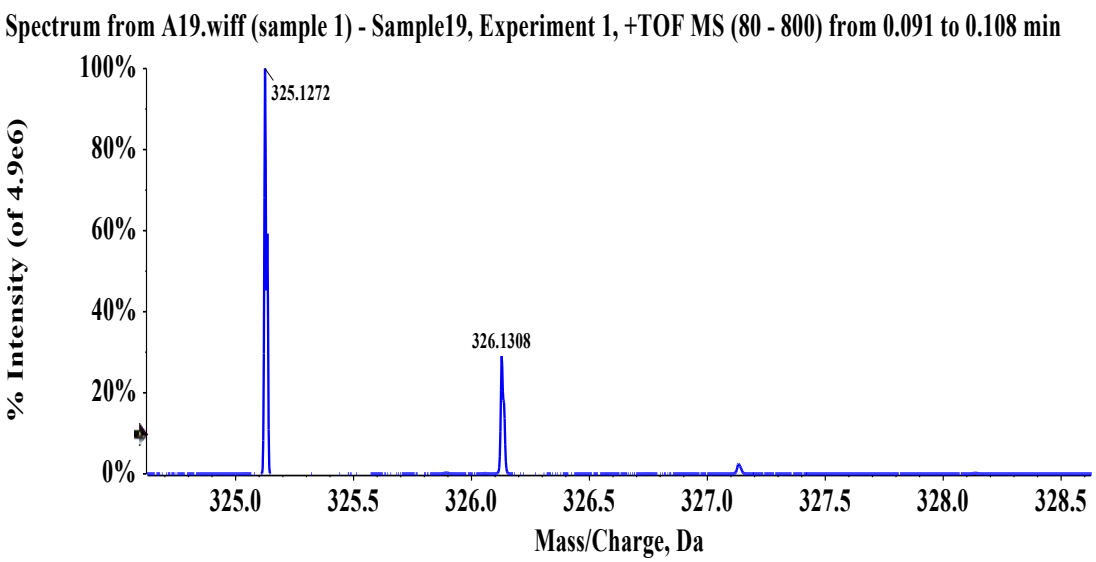

Figure 66. HRMS sprectrum of title compound 5t

Compound 5u

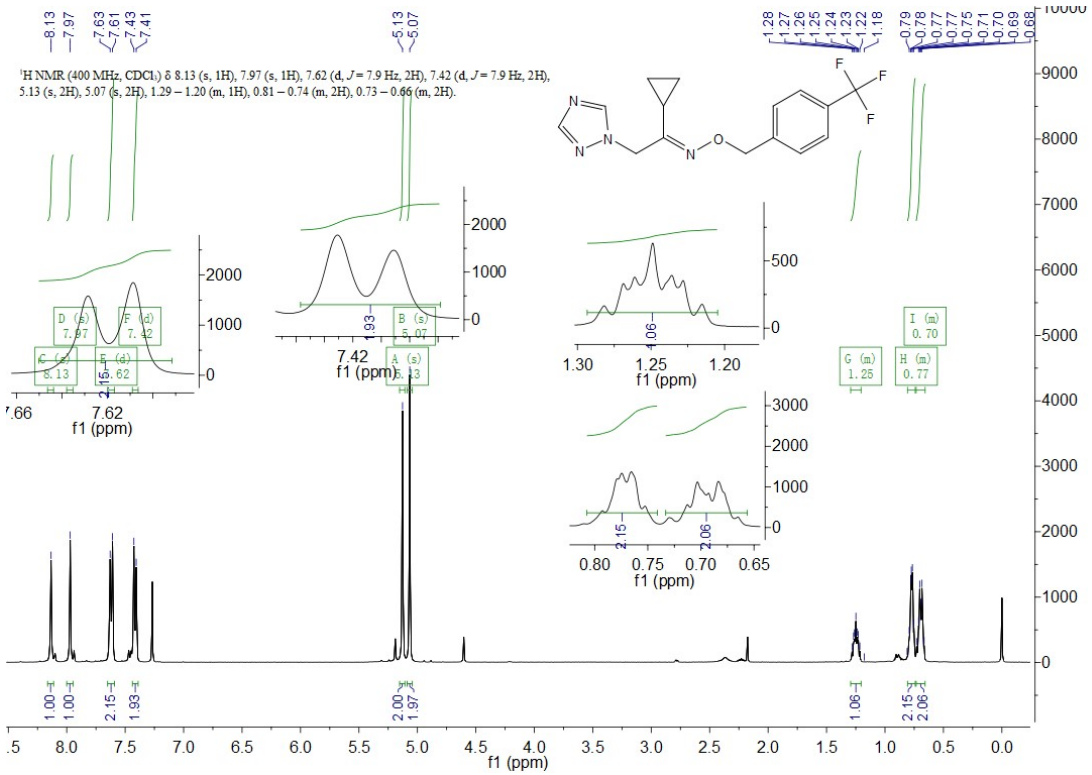

Figure 67. ^{1}H NMR sprectrum of title compound 5u

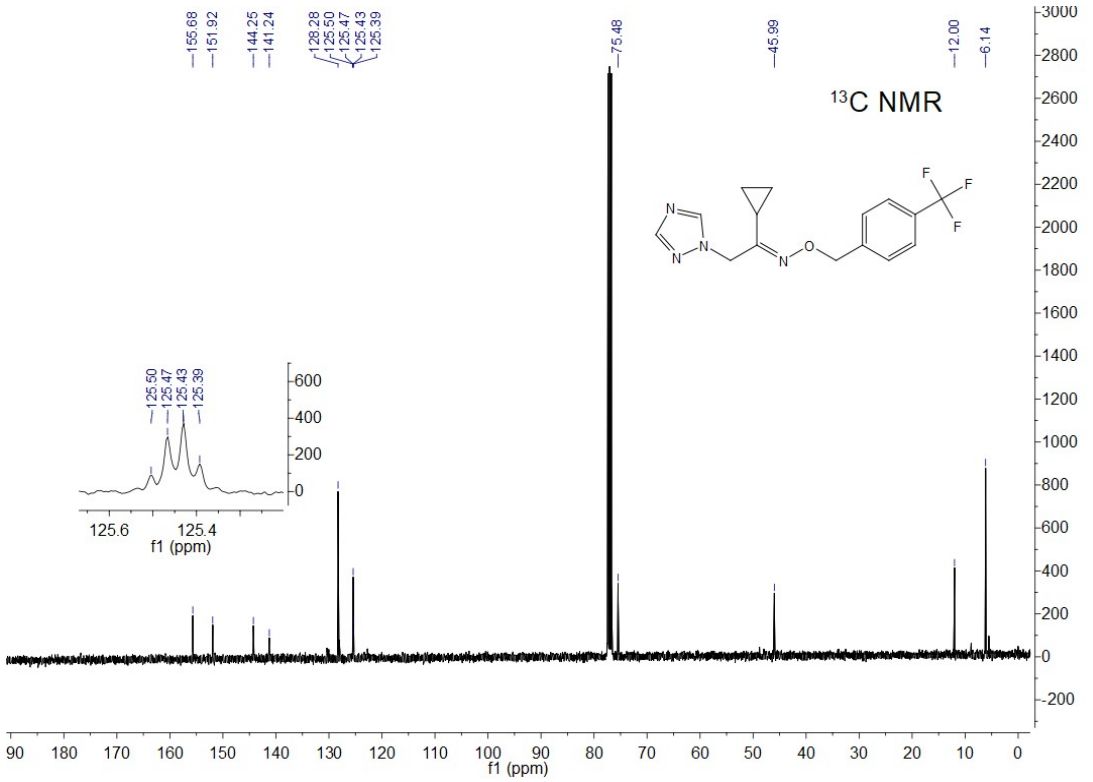

Figure 68. ^{13}C NMR sprectrum of title compound 5u

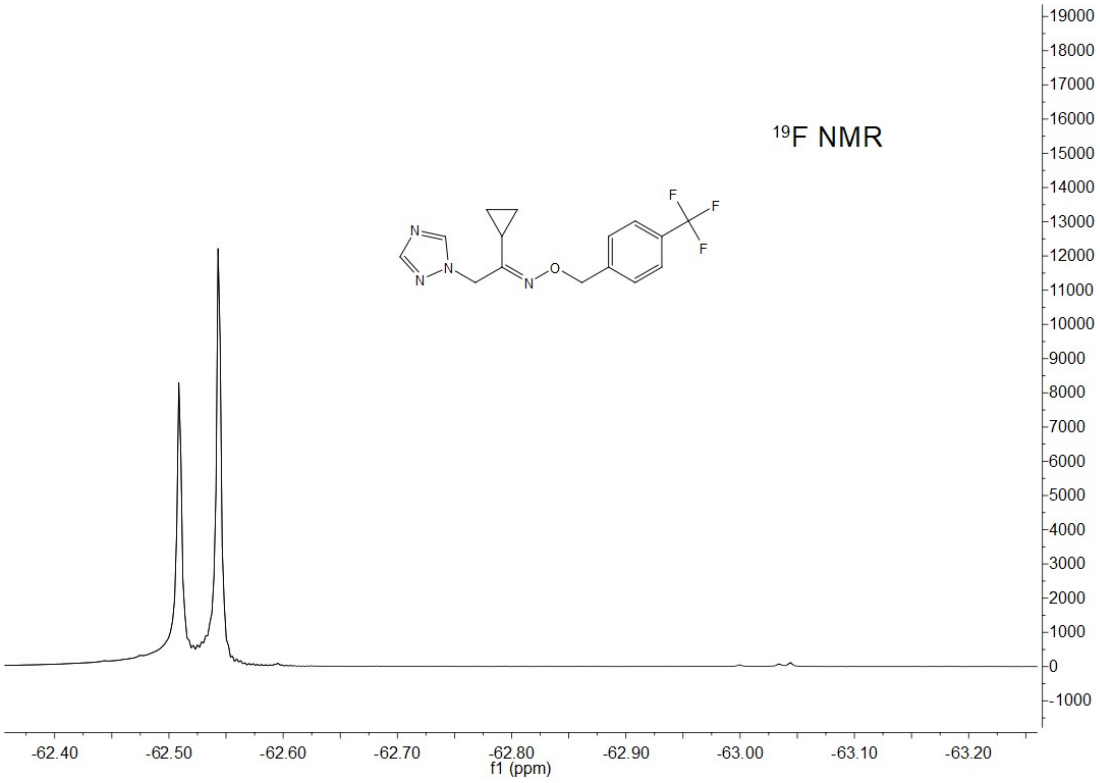

Figure 69. ^{19}F NMR sprectrum of title compound 5u

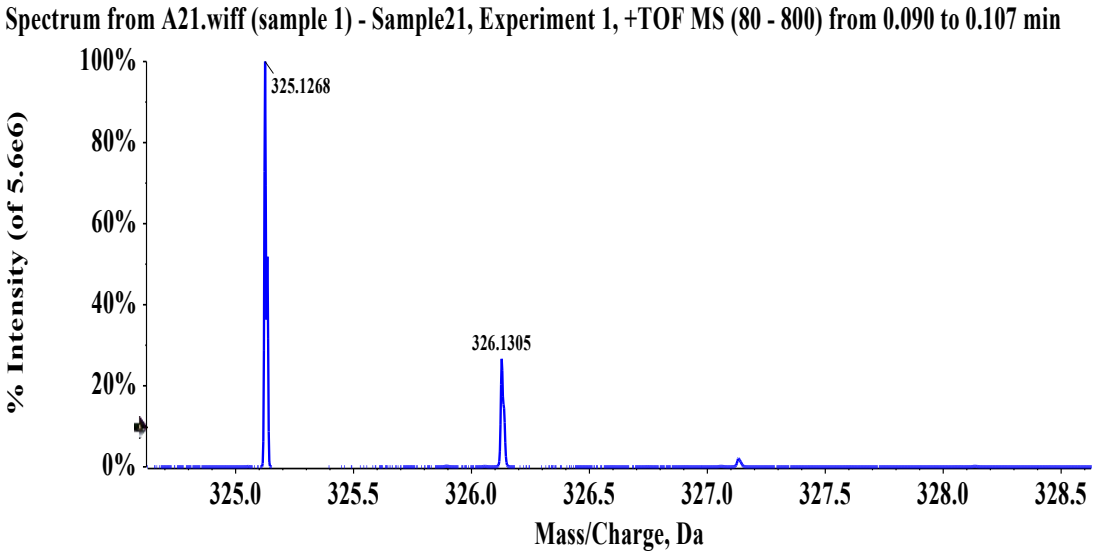

Figure 70. HRMS sprectrum of title compound 5u

Compound 5v

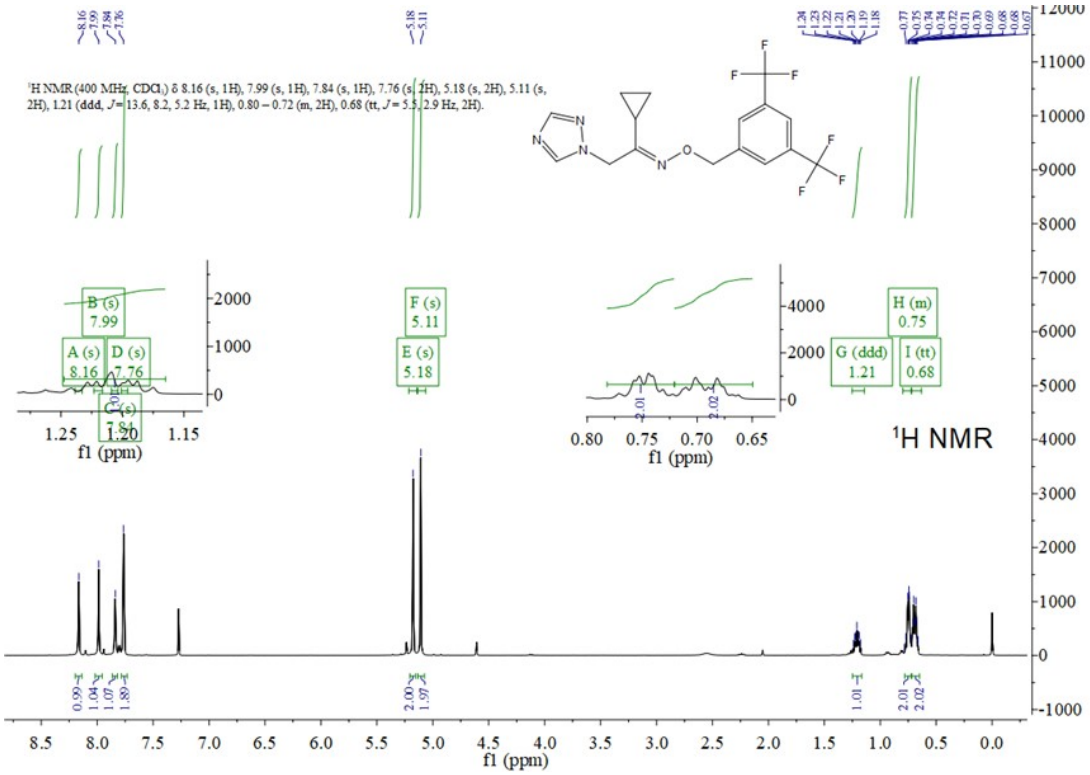

Figure 71. ^{1}H NMR sprectrum of title compound 5v

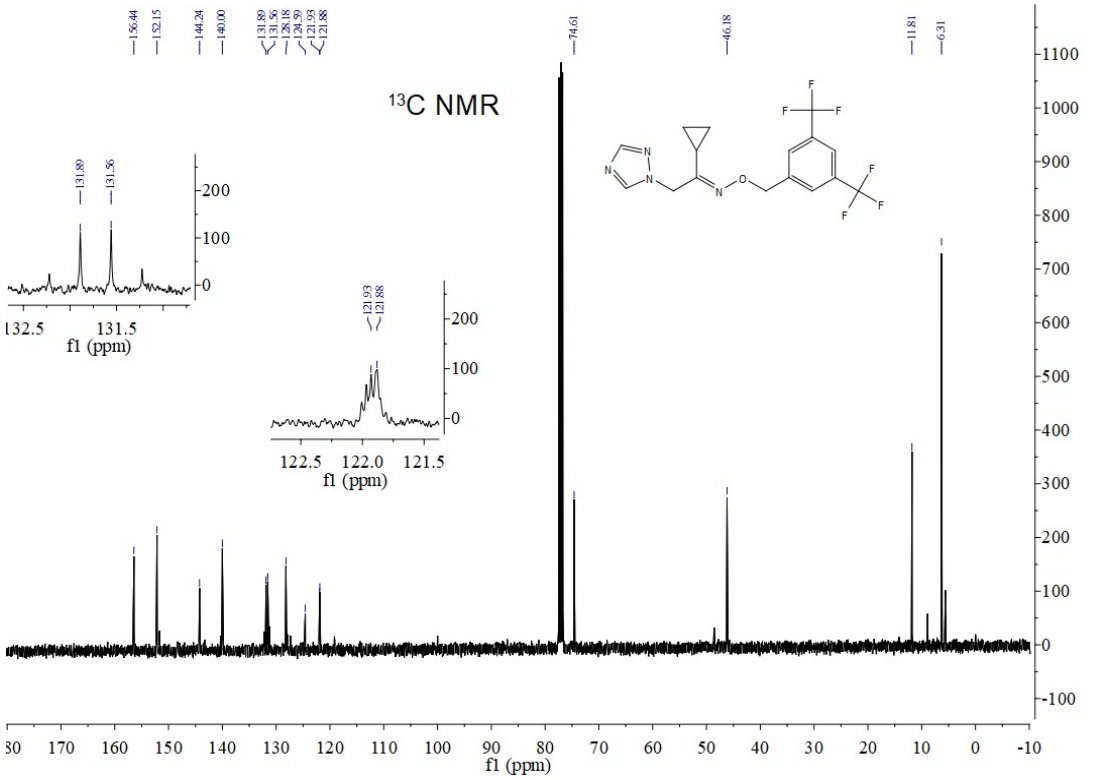

Figure 72. ^{13}C NMR sprectrum of title compound 5v

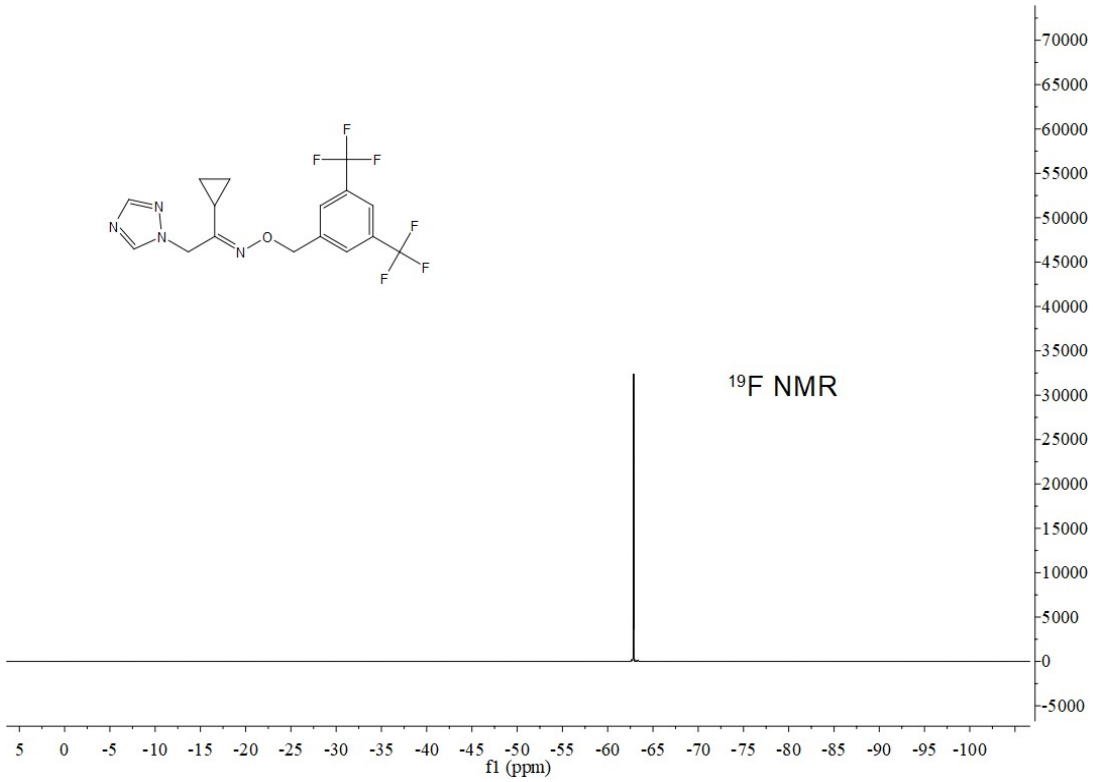

Figure 73. ^{19}F NMR sprectrum of title compound 5v

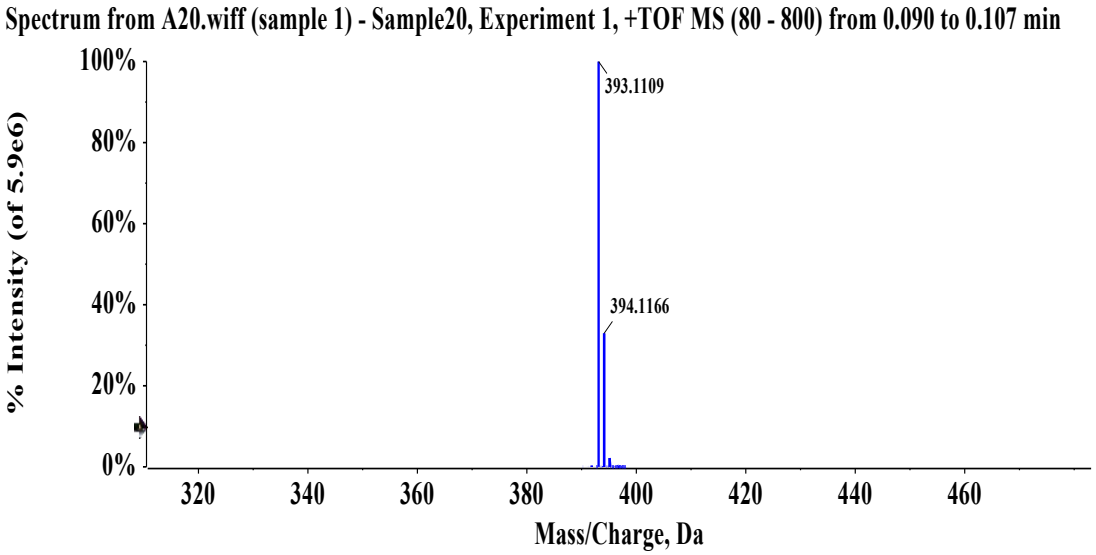

Figure 74. HRMS sprectrum of title compound 5v

Compound 5w

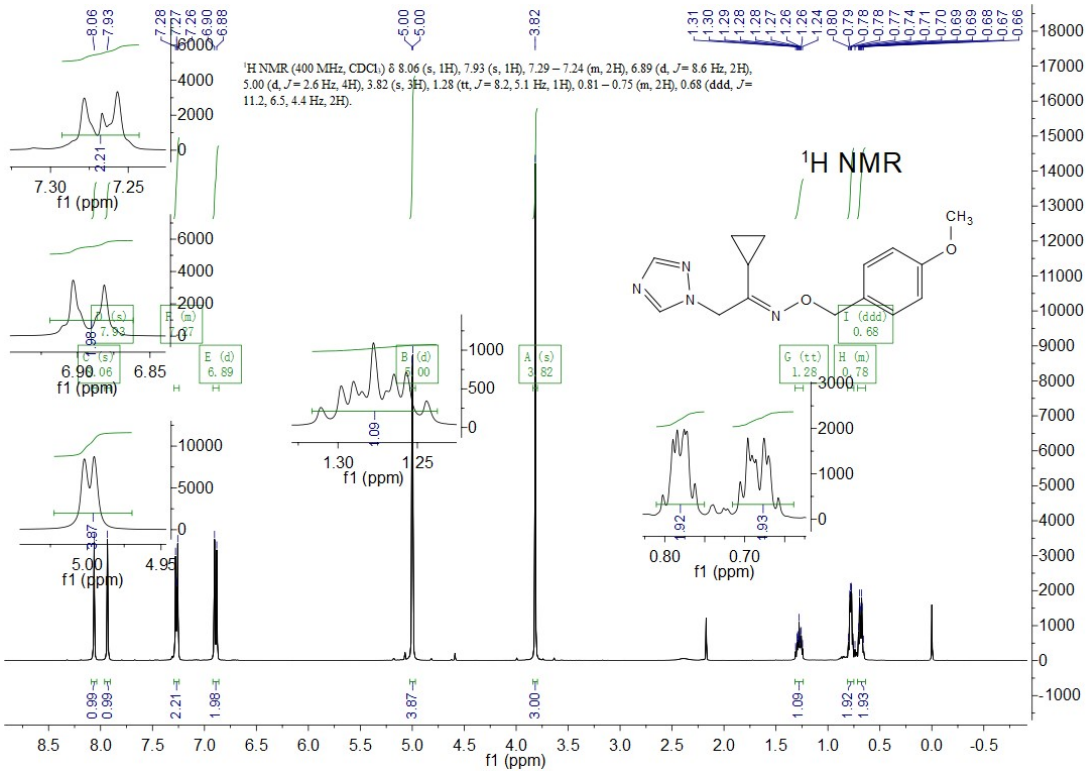

Figure 75. ^{1}H NMR sprectrum of title compound 5w

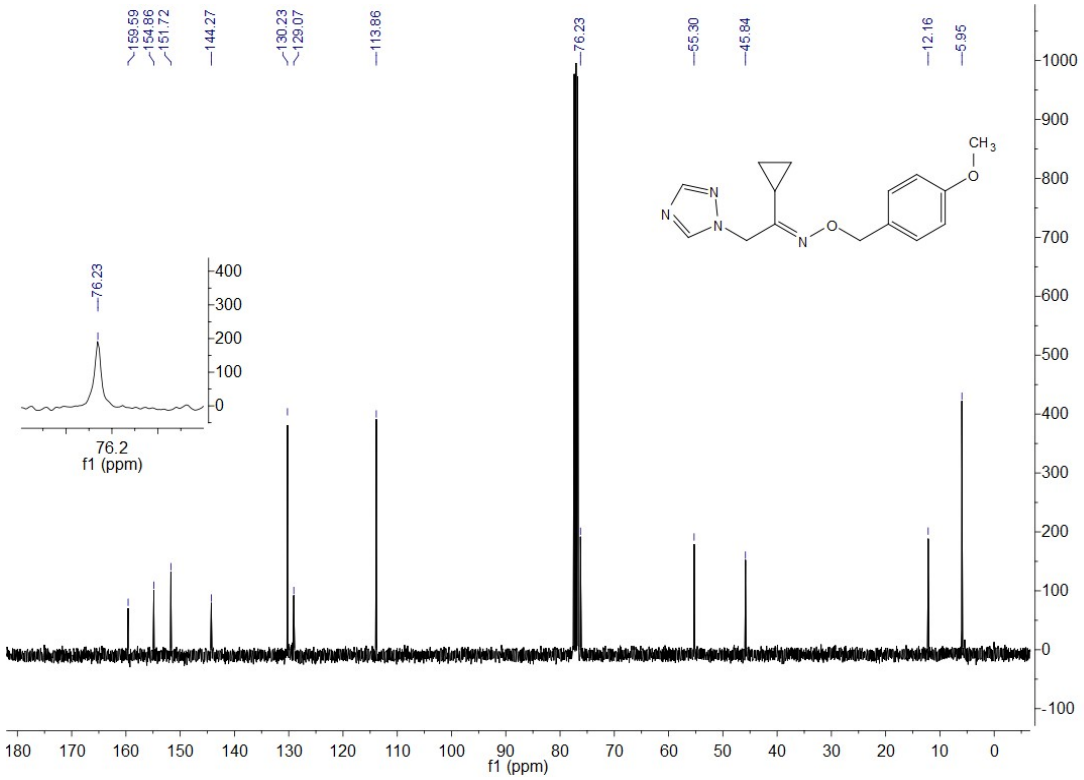

Figure 76. ^{13}C NMR sprectrum of title compound 5w

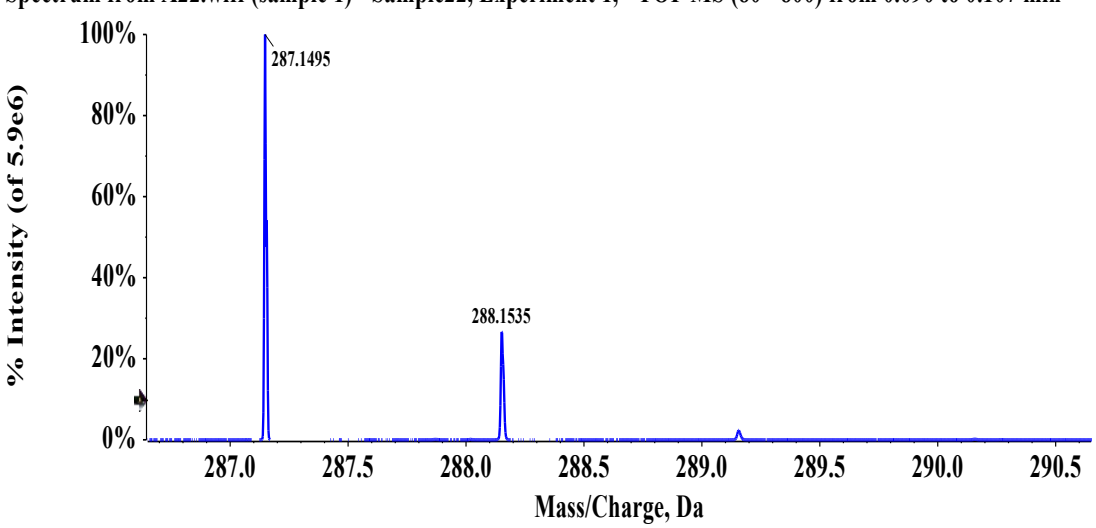

Figure 77. HRMS sprectrum of title compound 5w

Compound 5x

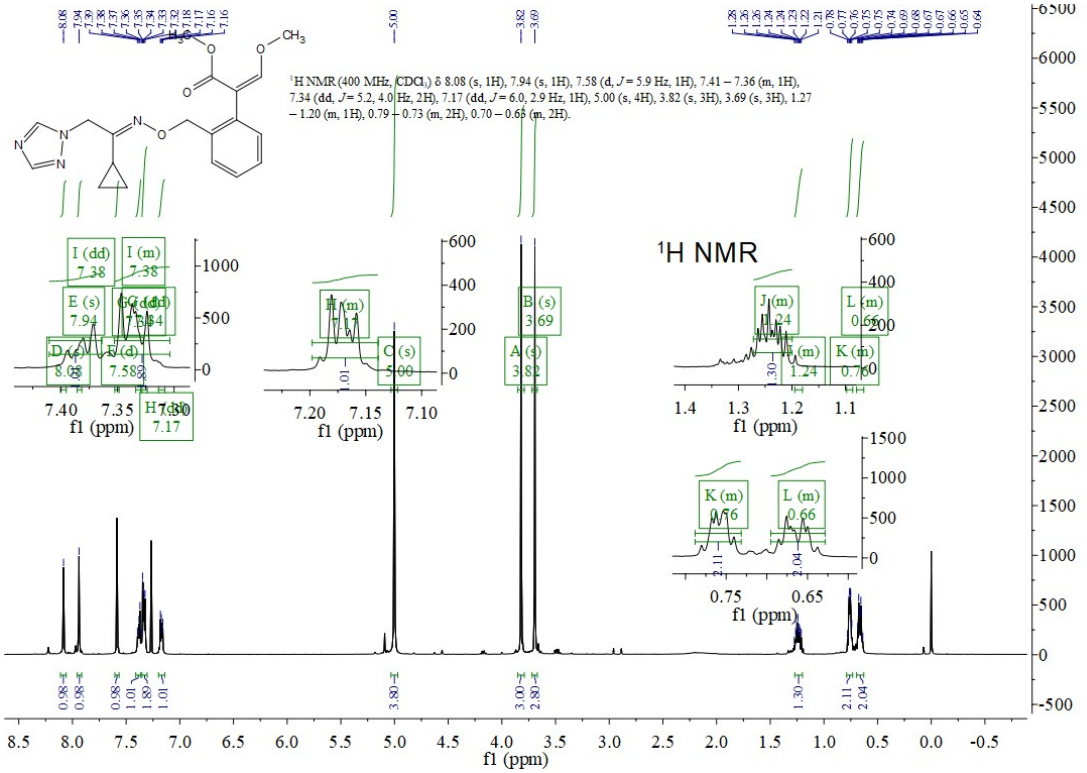

Figure 78. ^{1}H NMR sprectrum of intermediate 5x

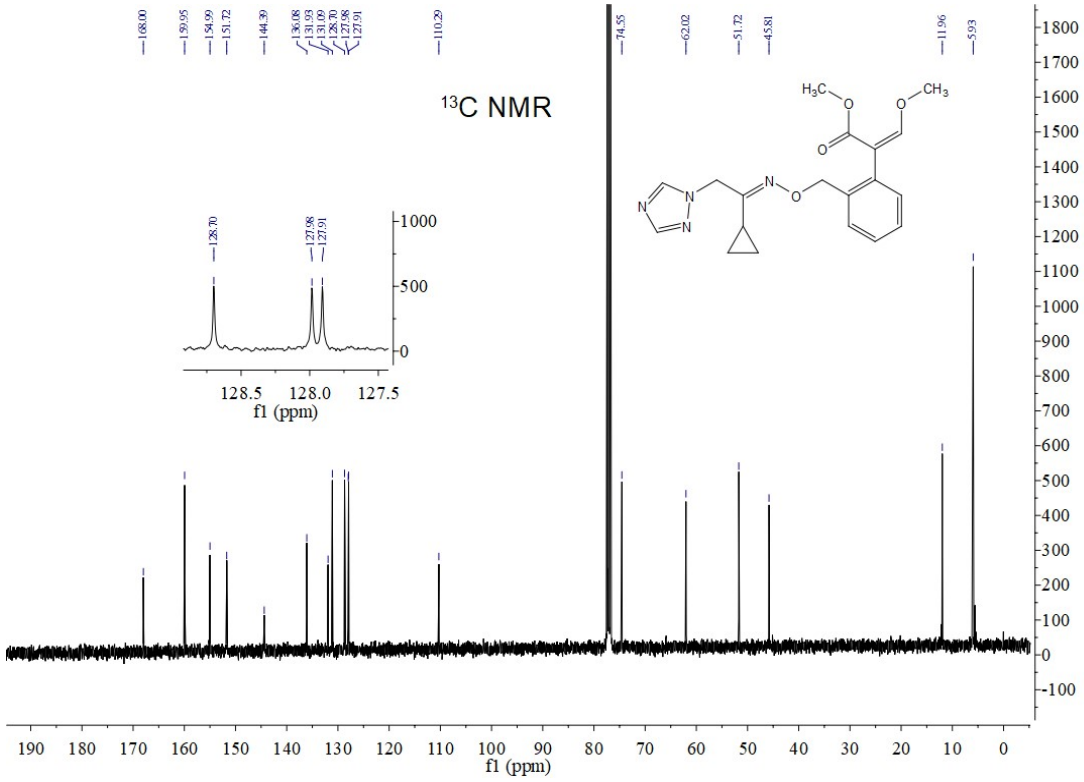

Figure 79. ^{13}C NMR sprectrum of title compound 5x

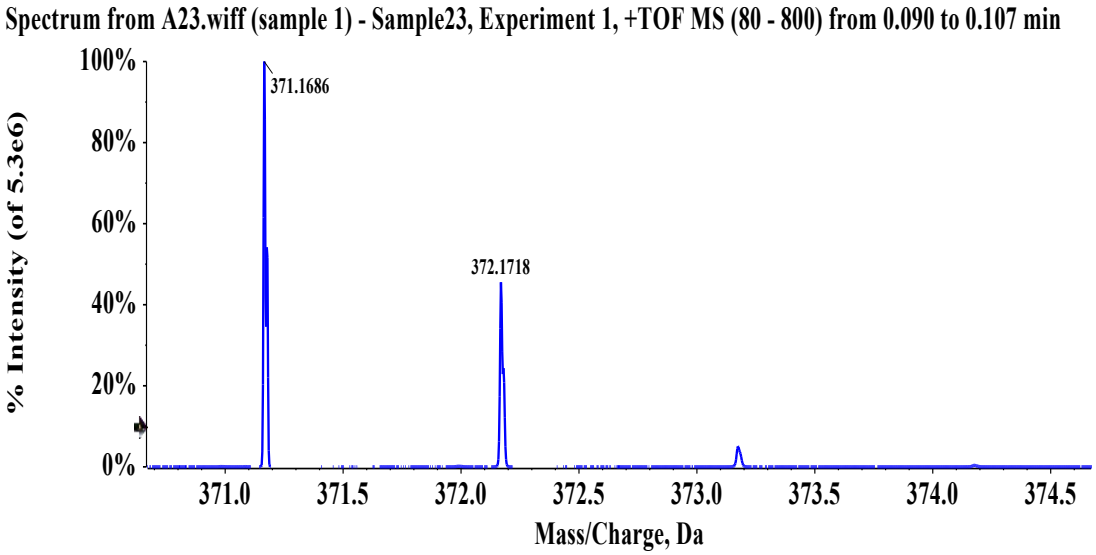

Figure 80. HRMS sprectrum of title compound 5x

2 Molecular docking related information

2.1 Protein sequence of *Fg*CYP51

>tr|I6YDU0|I6YDU0_GIBZA Cyp51A OS=Gibberella zeae OX=5518 PE=3 SV=1MFHLLIYPLWVLVALFAVIIANLLYQQLPRRPDEPPLVFHWFPFFGNAVAYGLDPCG FFEKCREKHGDVFTFILFGRKIVACLGVDGNDFVLNSRLQDANAEEVYGPLTIPVFGSDV VYDCPNSKLMEQKKFVKFGLTQKALESHVQLIEREVLDYVETDPSFSGRTSTIDVPKAMA EITIFTASRSLQGEEVRRKLTAEFAALYHDLDLGFRPVNFLFPWLPLPHNRKRDAAHIKMR EVYMDIINDRRKGGIRTEDGTDMIANLMGCTYKNGQPVPDKEIAHMMITLLMAGQHSSS SASSWIVLHLASSPDMTEELYQEQLVNLSVNGALPPLQYSDLDKLPLLQNVVKETLRVHS SIHSILRKVKRPMQVPNSPYTITTDKVIMASPTVTAMSEEYFENAKTWNPHRWDNRAKEE VDTEDVIDYGYGAVSKGTKSPYLPFGAGRHRCIGEKFAYVNLGVIVATLVRNFRLSTIDG RPGVPETDYTSLFSRPAQPAFIRWERRKKI

2.2 Ramachandran plots of constructed protein *Fg*CYP51

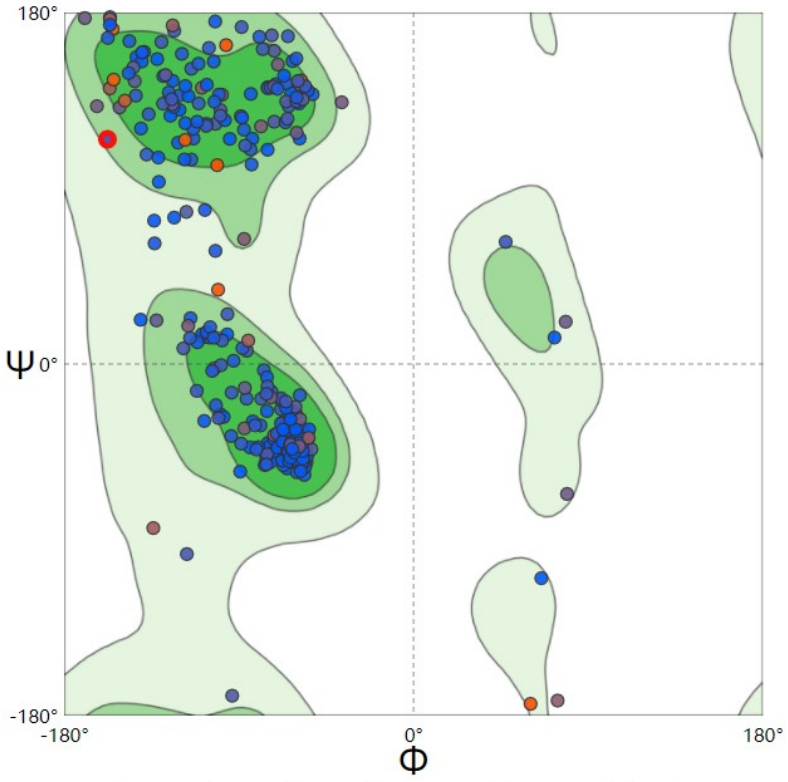

Figure 81. Ramachandran plots of constructed protein *Fg*CYP51

2.3 Composite image of 4YUM and constructed protein *Fg*CYP51

Figure 82. Composite image of 4yum (blue) and constructed protein (purple) *Fg*CYP51

2.4 Molecular docking diagram of compound (*E*)-5k and (*S*)-tebuconazole

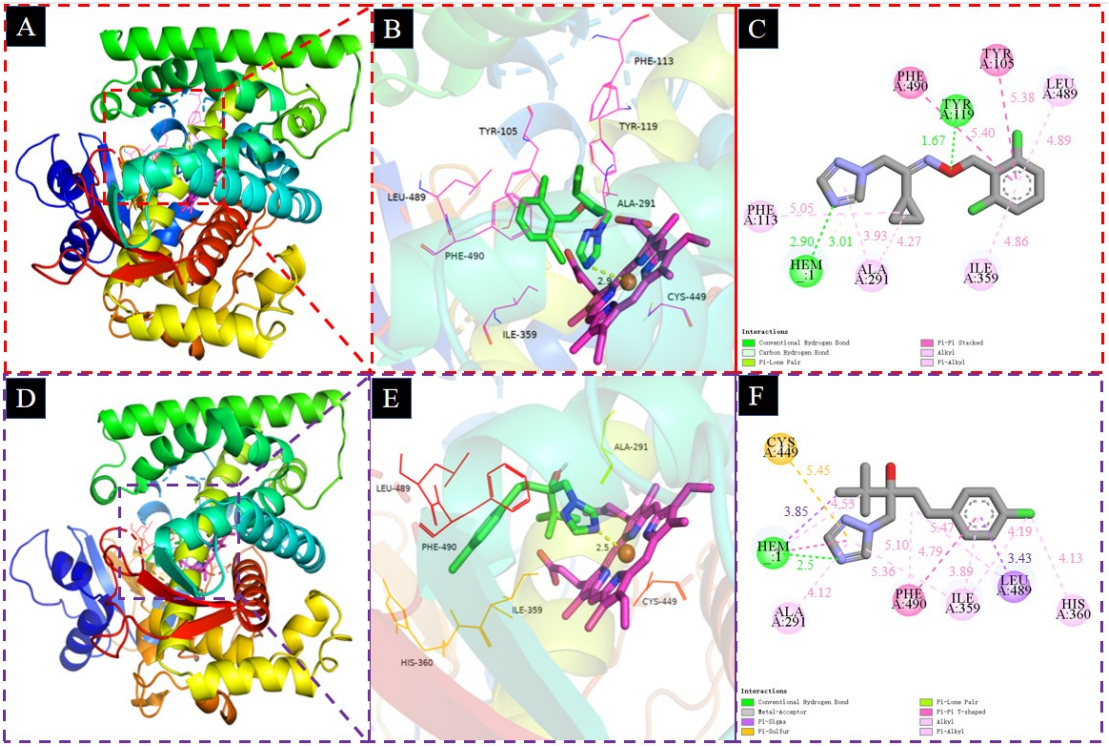

Figure 83. Molecular docking diagram of compound (*E*)-5k (A−C) and (*S*)-tebuconazole (D−F)