

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

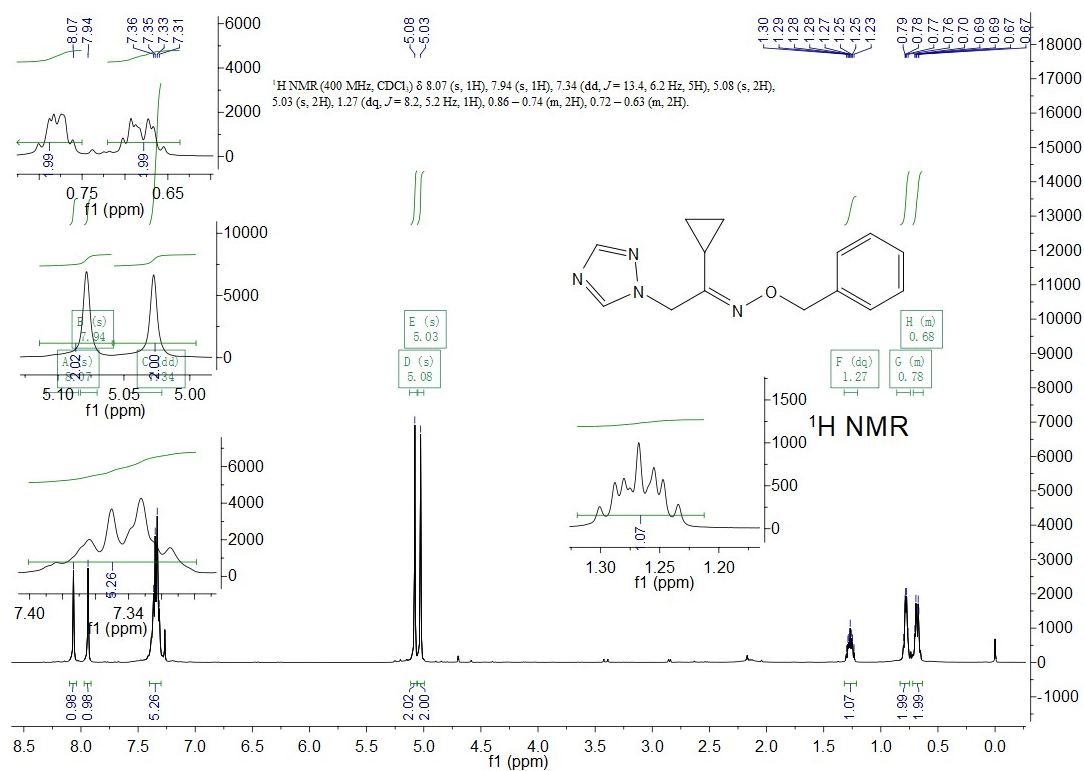


Figure 1. ¹H NMR spectrum of title compound 5a

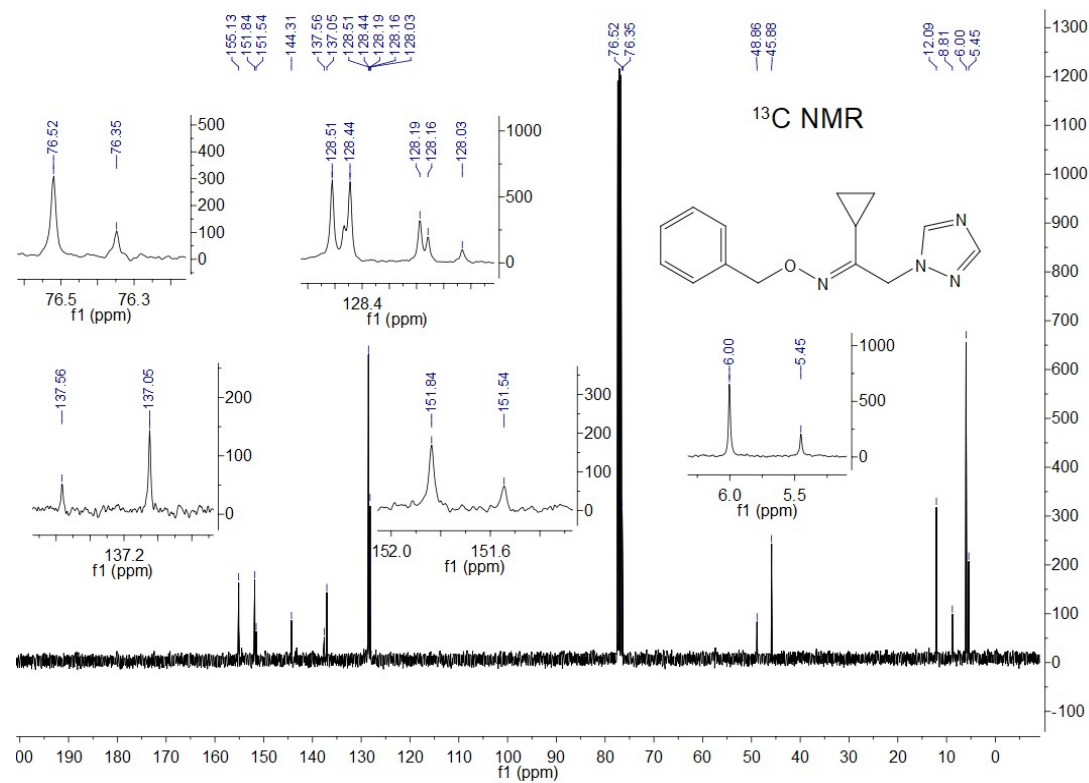


Figure 2. ¹³C NMR spectrum of title compound 5a

Spectrum from A01.wiff (sample 1) - Sample01, Experiment 1, +TOF MS (80 - 800) from 0.072 to 0.081 min

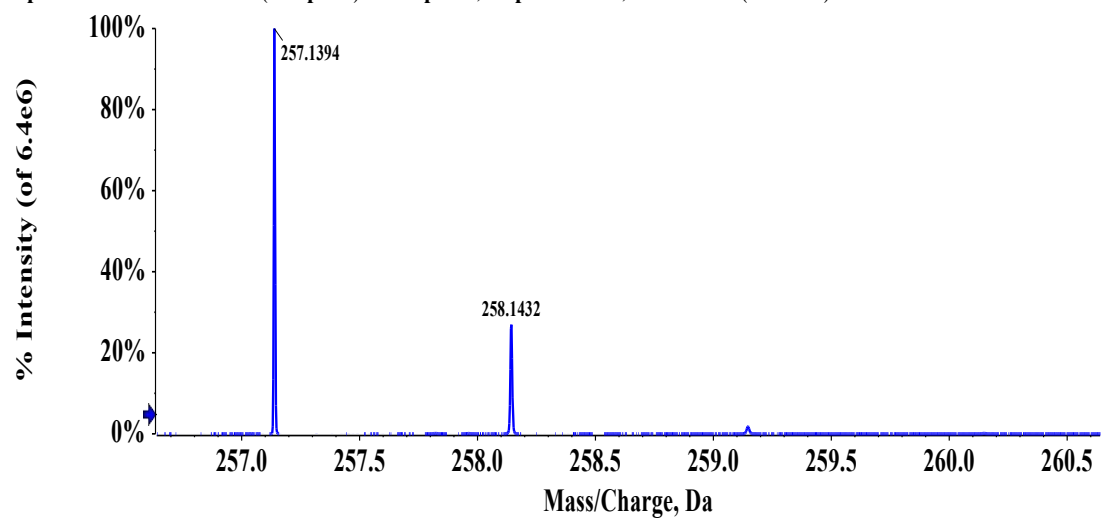


Figure 3. HRMS spectrum of title compound 5a

Compound 5b

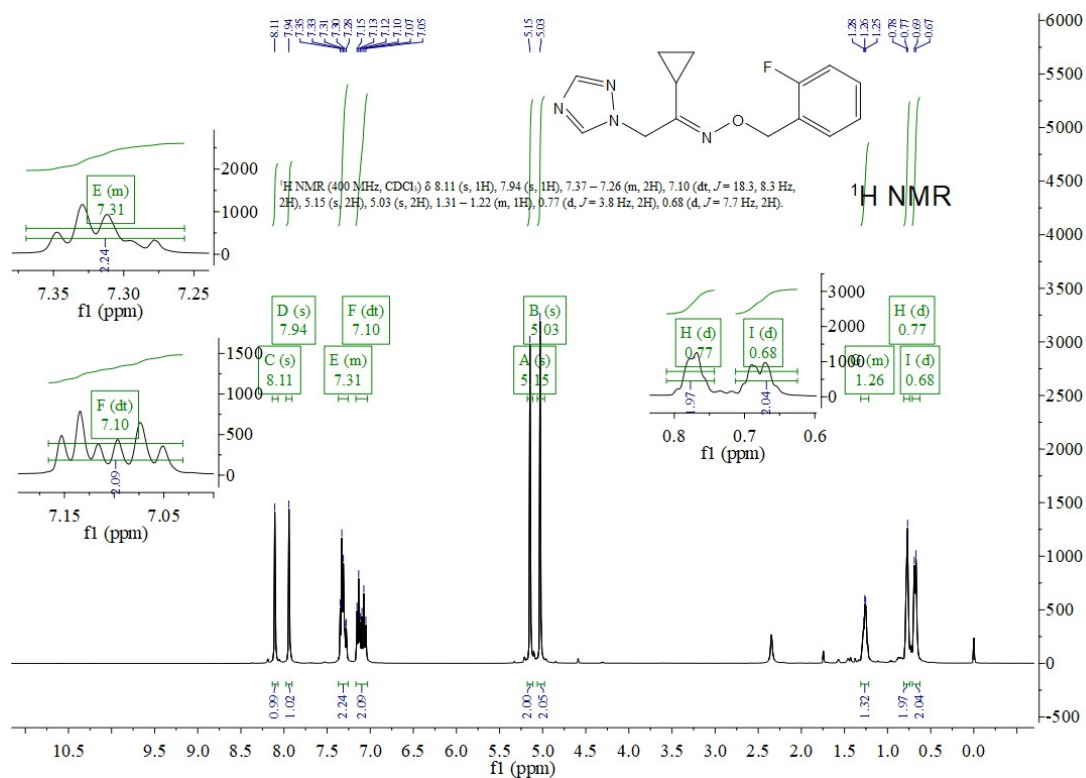


Figure 4. ¹H NMR spectrum of title compound 5b

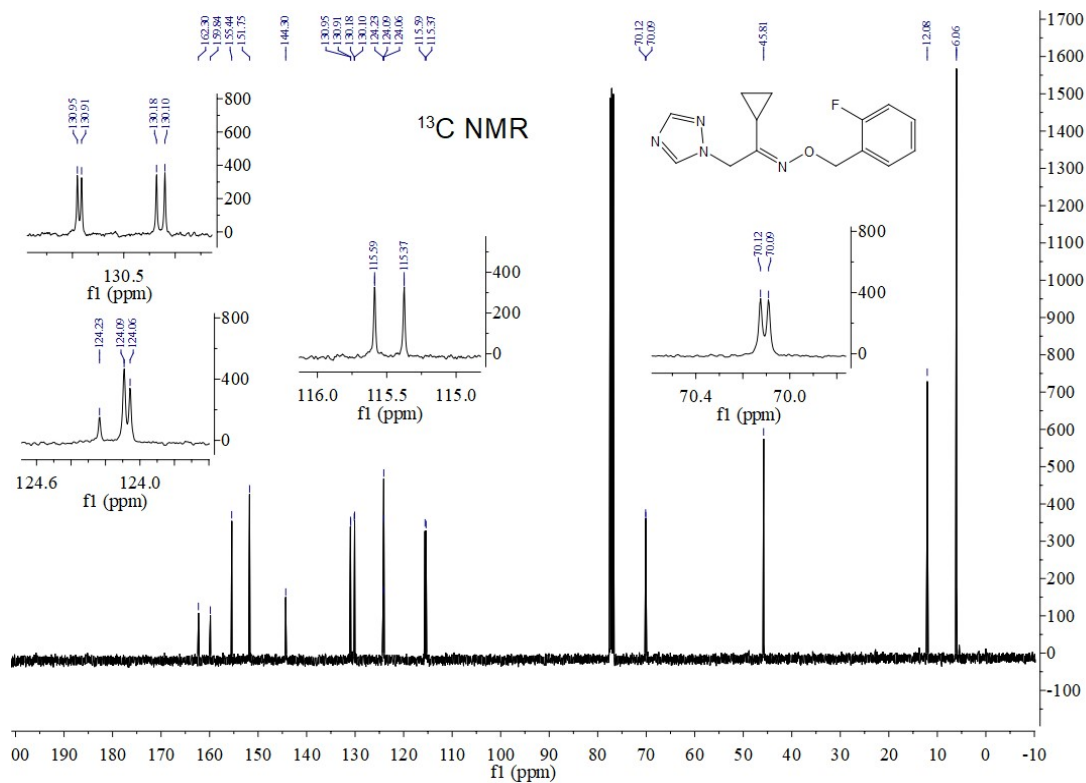


Figure 5. ¹³C NMR spectrum of title compound 5b

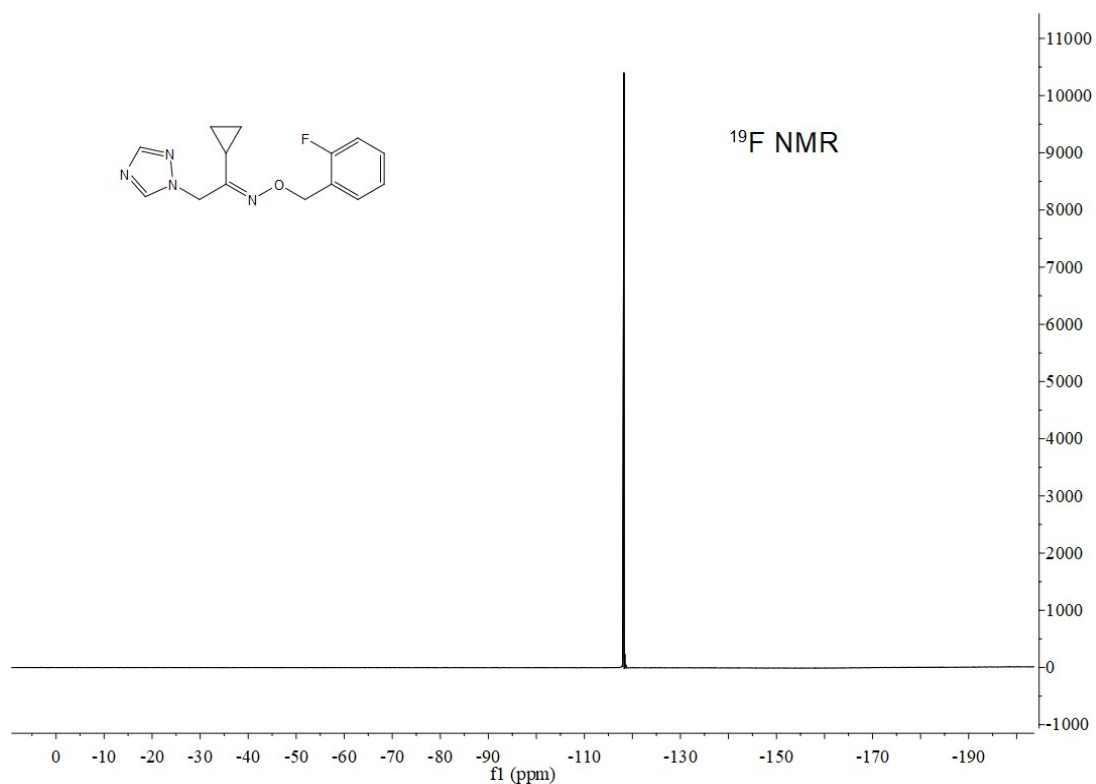


Figure 6. ^{19}F NMR spectrum of title compound 5b

Spectrum from A02.wiff (sample 1) - Sample02, Experiment 1, +TOF MS (80 - 800) from 0.085 to 0.094 min

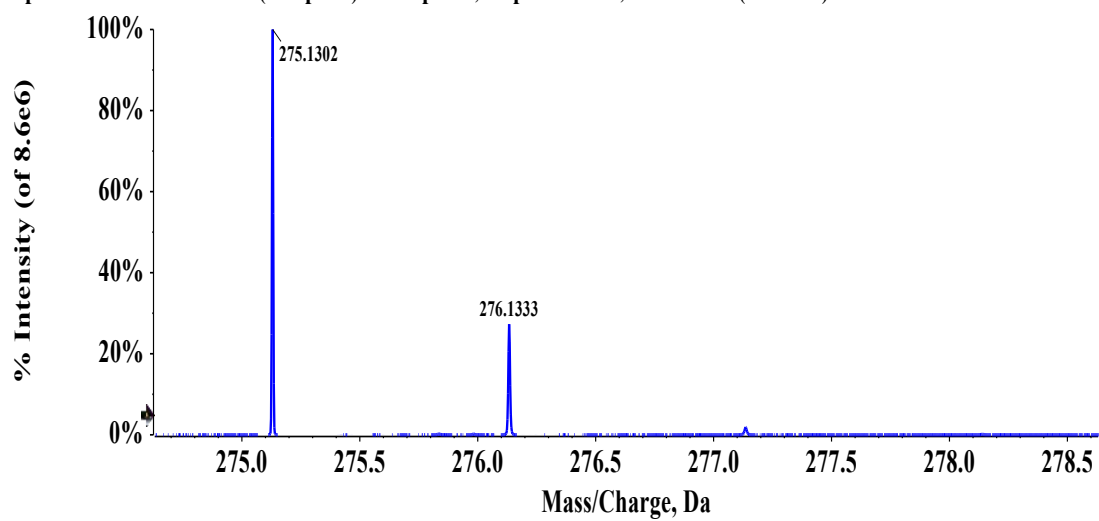


Figure 7. HRMS spectrum of title compound 5b

Compound 5c

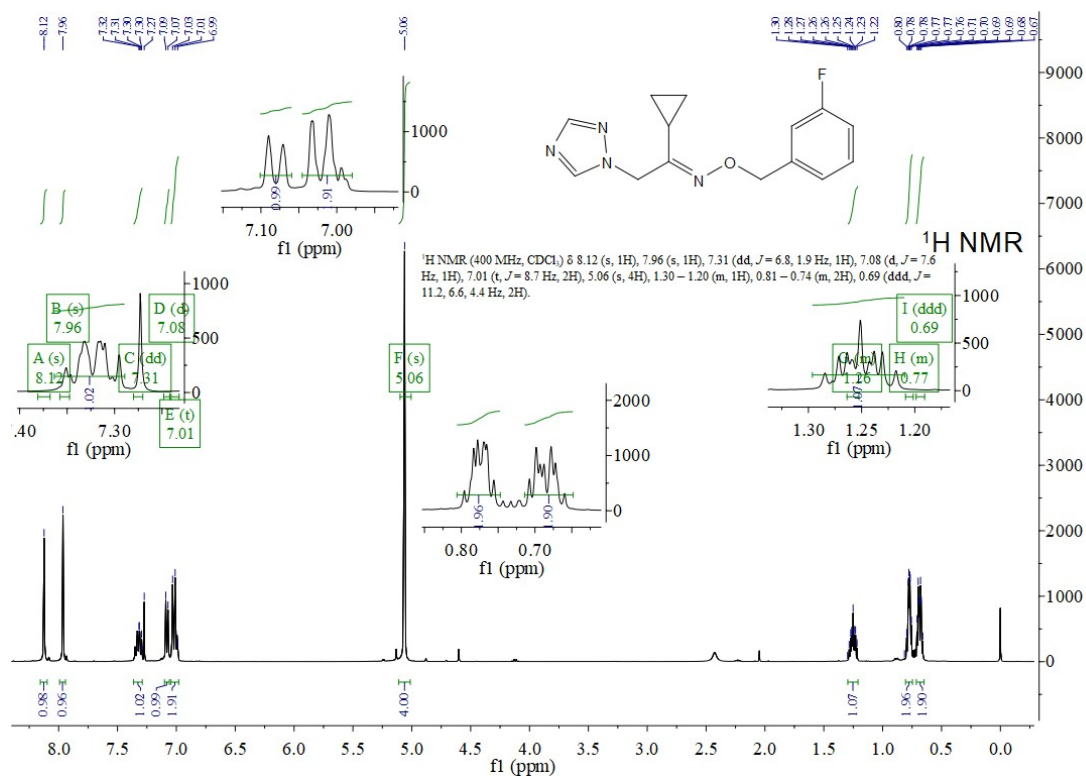


Figure 8. ¹H NMR spectrum of title compound 5c

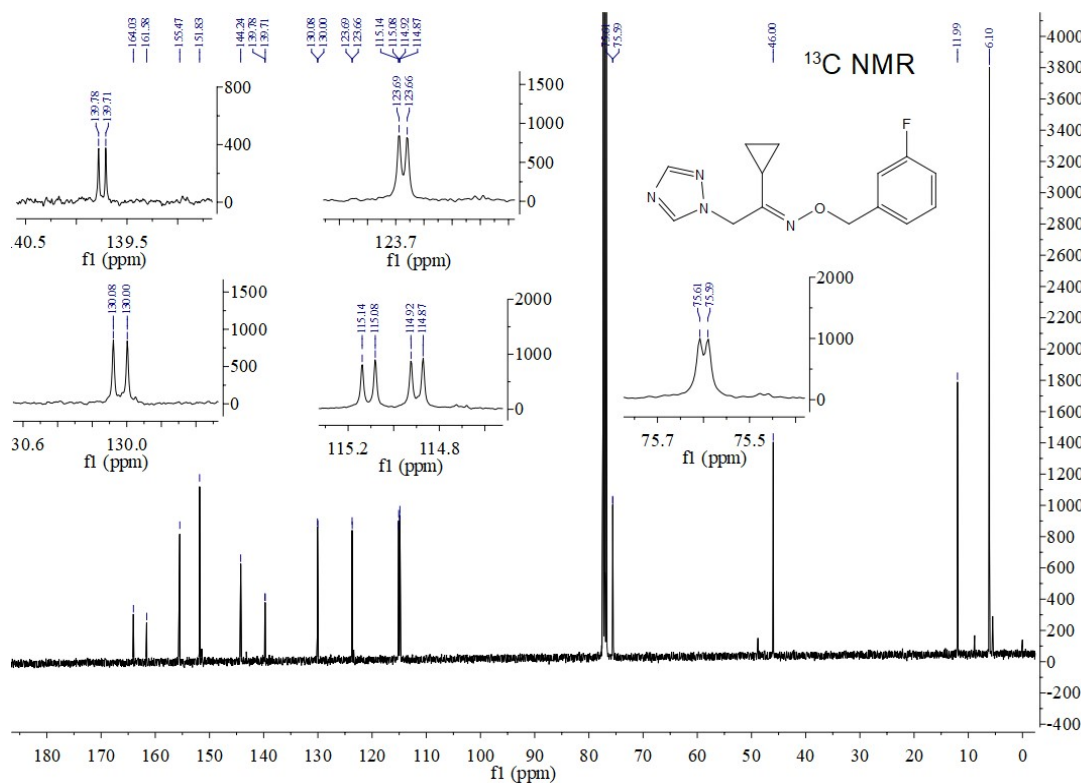


Figure 9. ¹³C NMR spectrum of title compound 5c

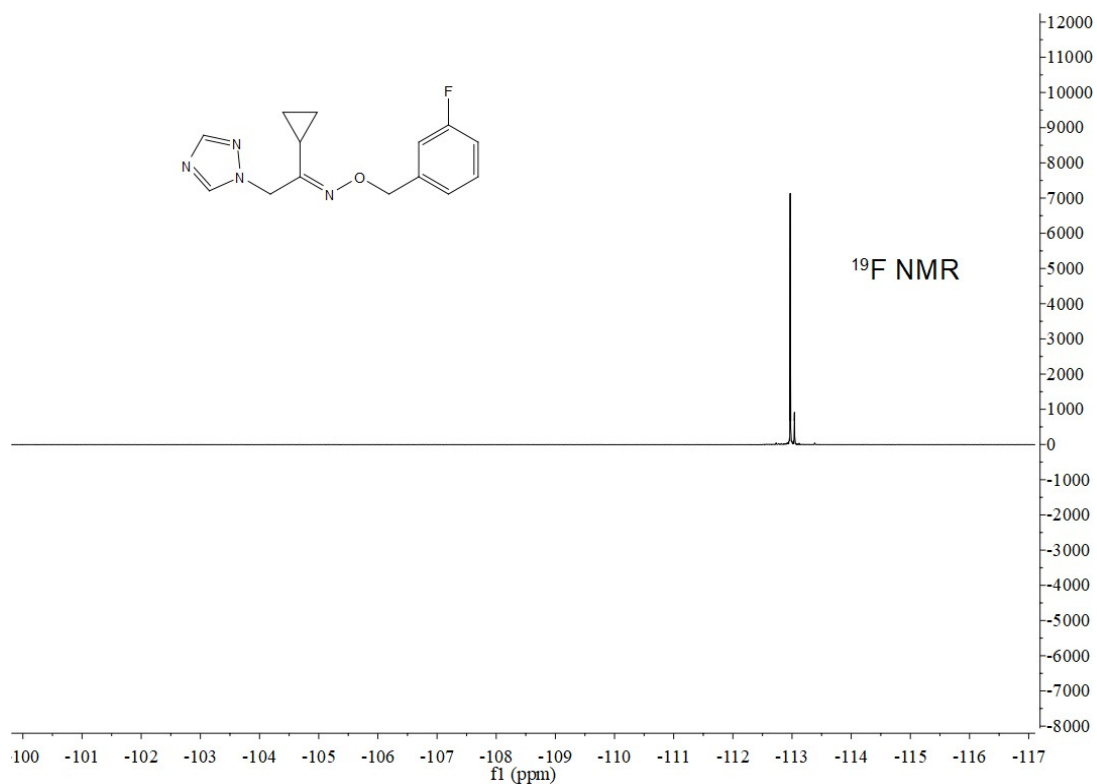


Figure 10. ¹⁹F NMR spectrum of title compound 5c

Spectrum from A02.wiff (sample 1) - Sample02, Experiment 1, +TOF MS (80 - 800) from 0.085 to 0.094 min

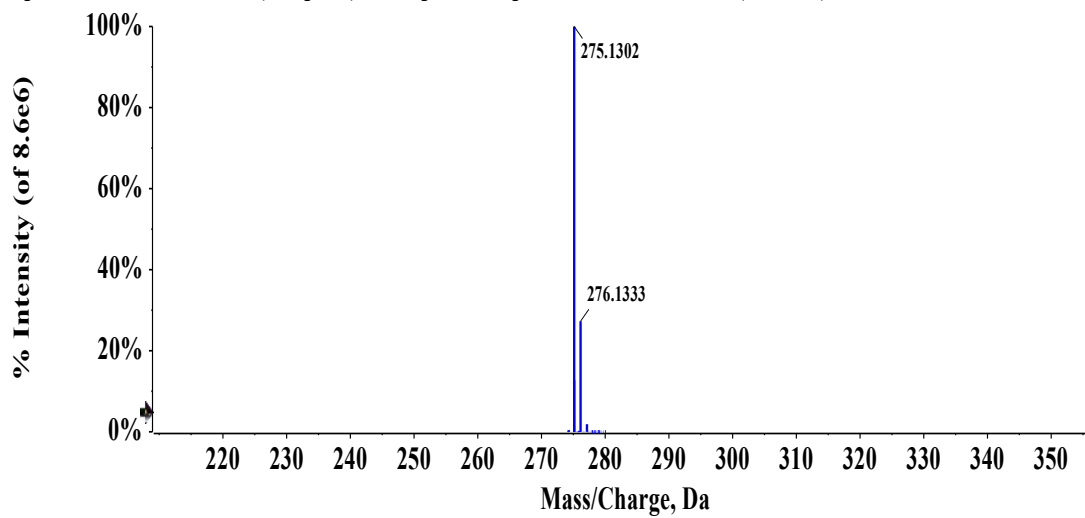


Figure 11. HRMS spectrum of title compound 5c

Compound 5d

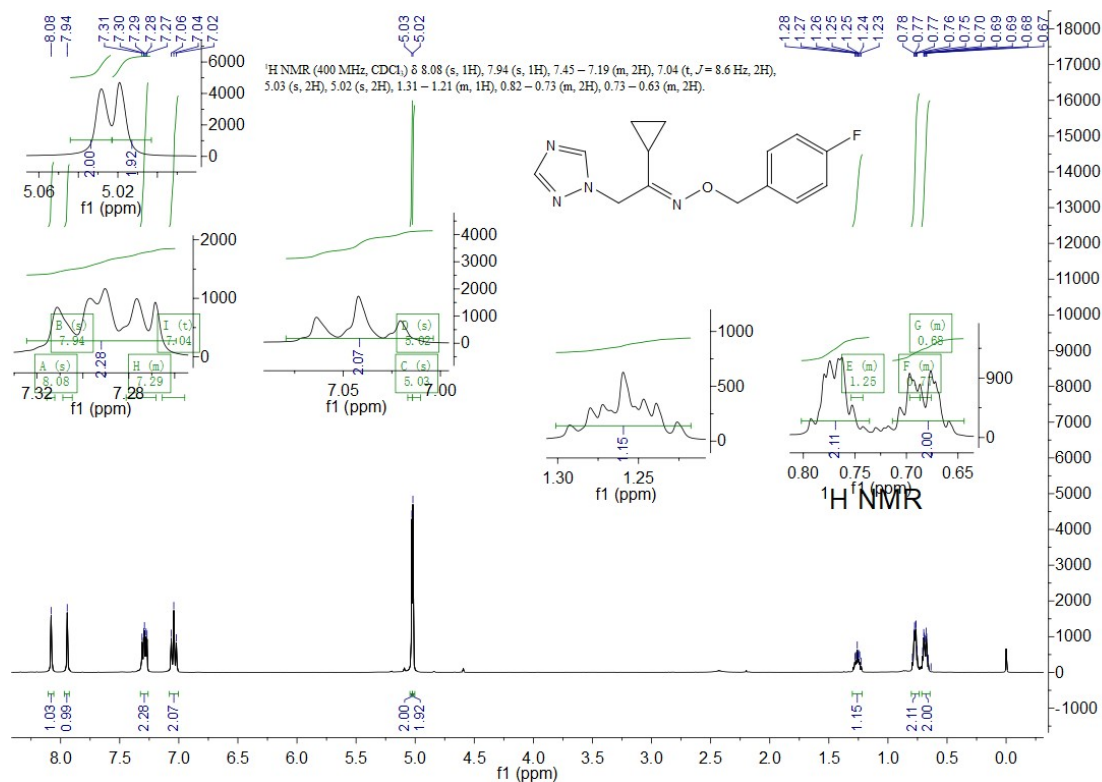


Figure 12. ¹H NMR spectrum of title compound 5d

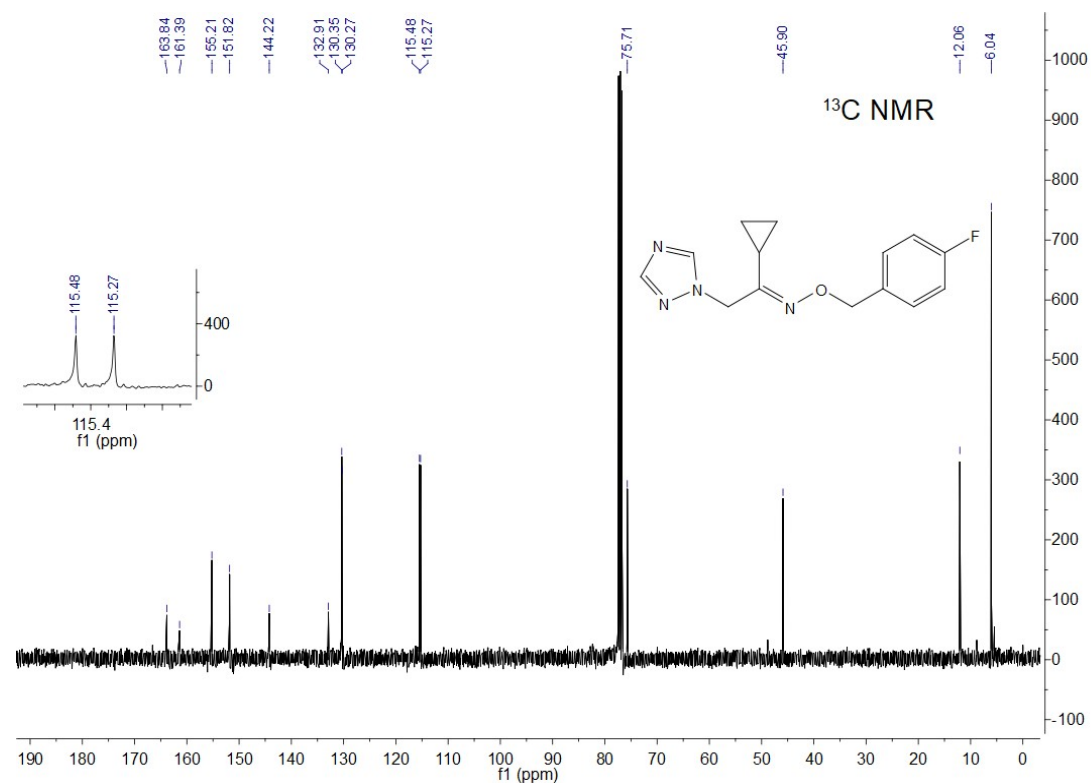


Figure 13. ¹³C NMR spectrum of title compound 5d

Spectrum from A04.wiff (sample 1) - Sample04, Experiment 1, +TOF MS (80 - 800) from 0.072 to 0.082 min

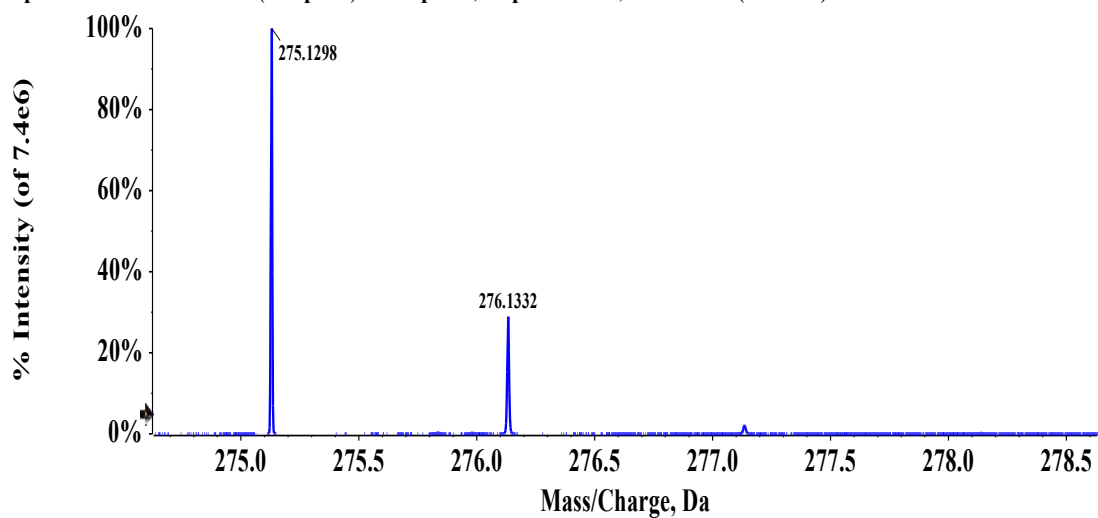


Figure 14. HRMS spectrum of title compound 5d

Compound 5e

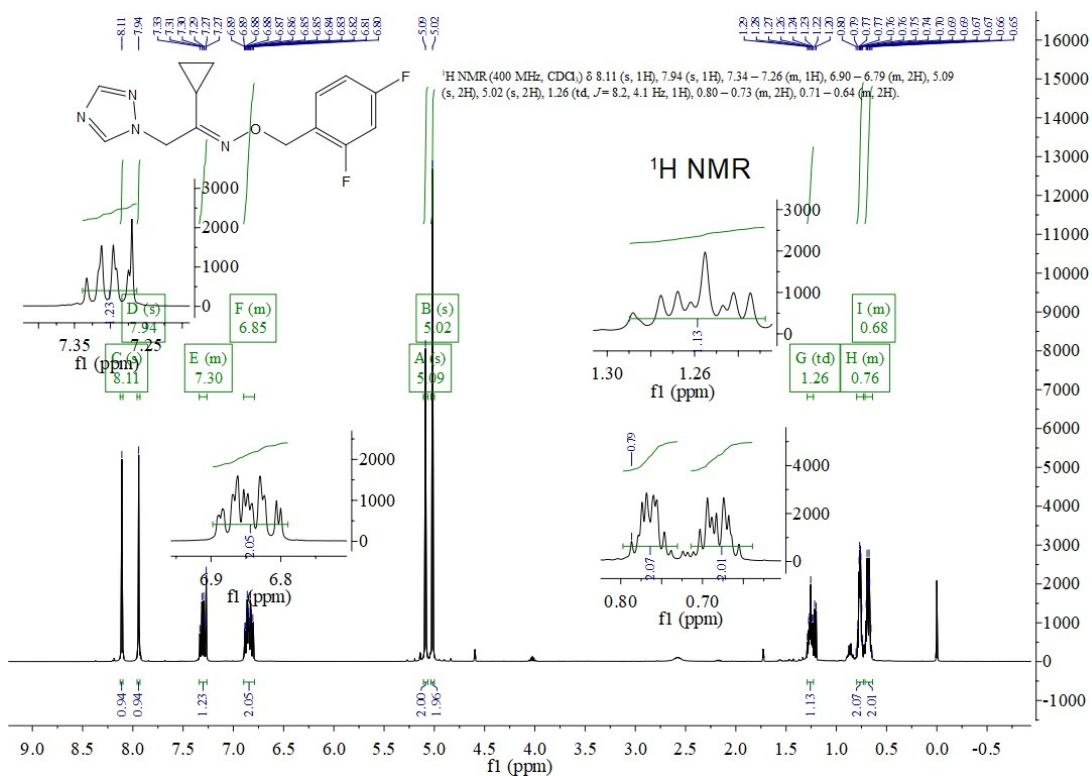


Figure 15. ¹H NMR spectrum of title compound 5e

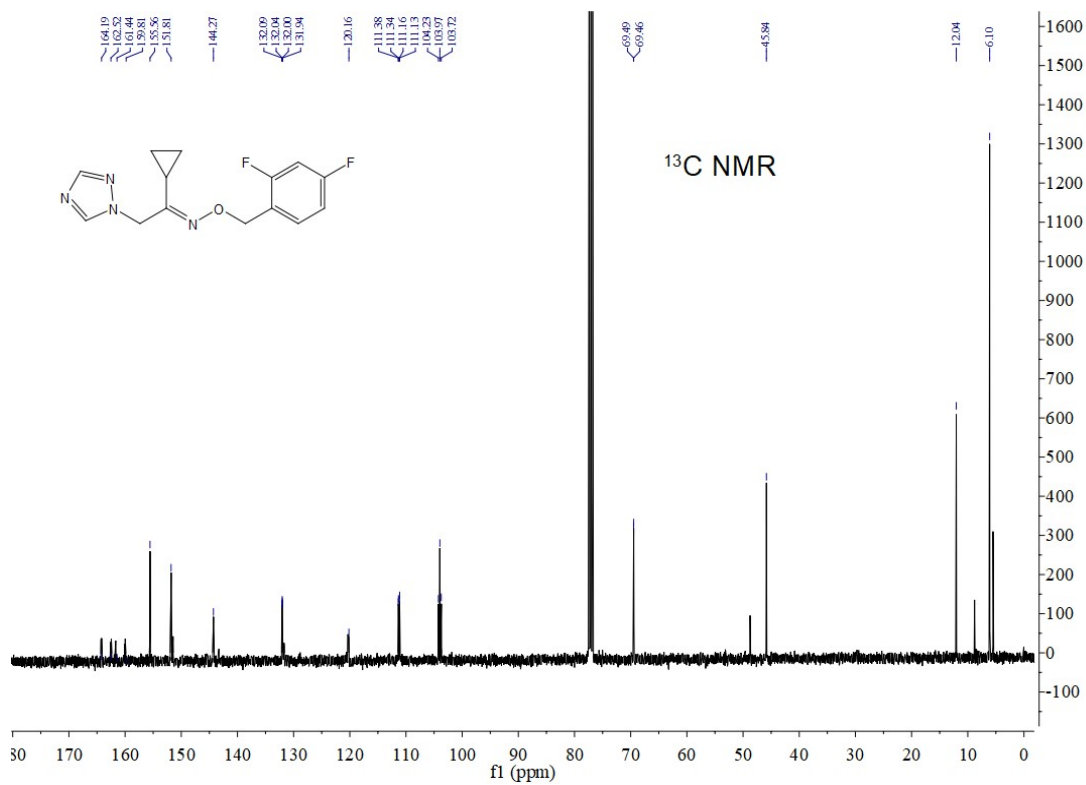


Figure 16. ¹³C NMR spectrum of title compound 5e

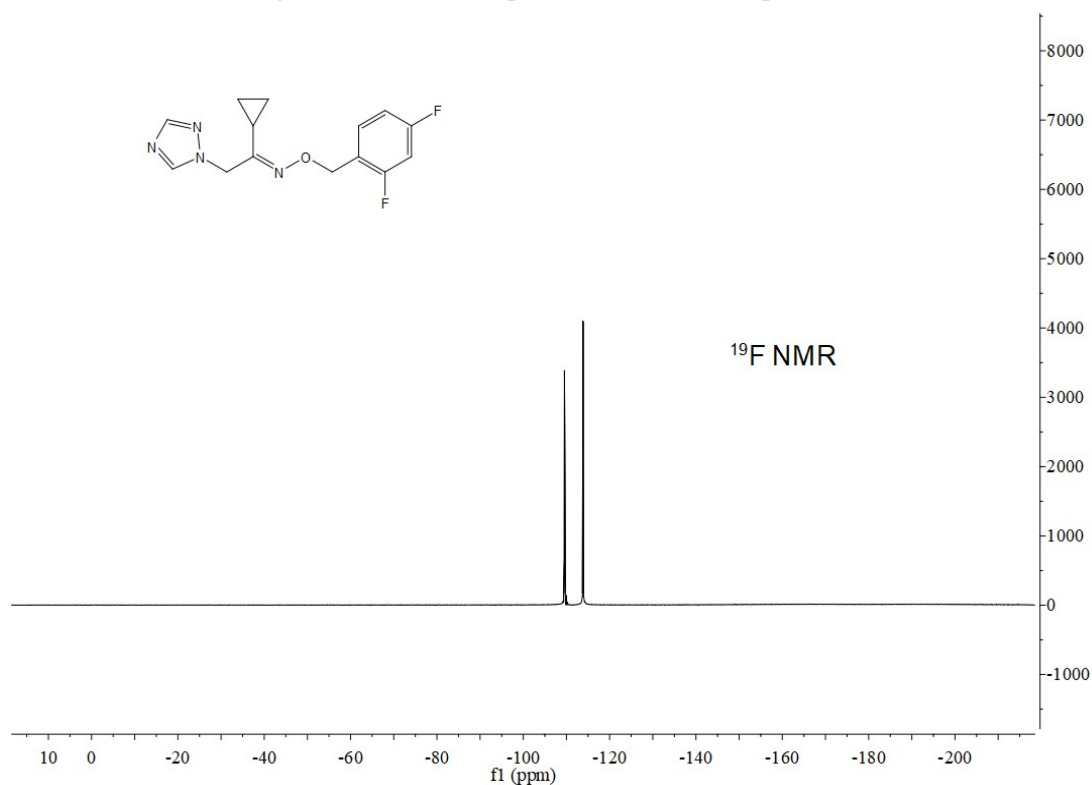


Figure 17. ¹⁹F NMR spectrum of title compound 5e

Spectrum from A05.wiff (sample 1) - Sample05, Experiment 1, +TOF MS (80 - 800) from 0.085 to 0.094 min

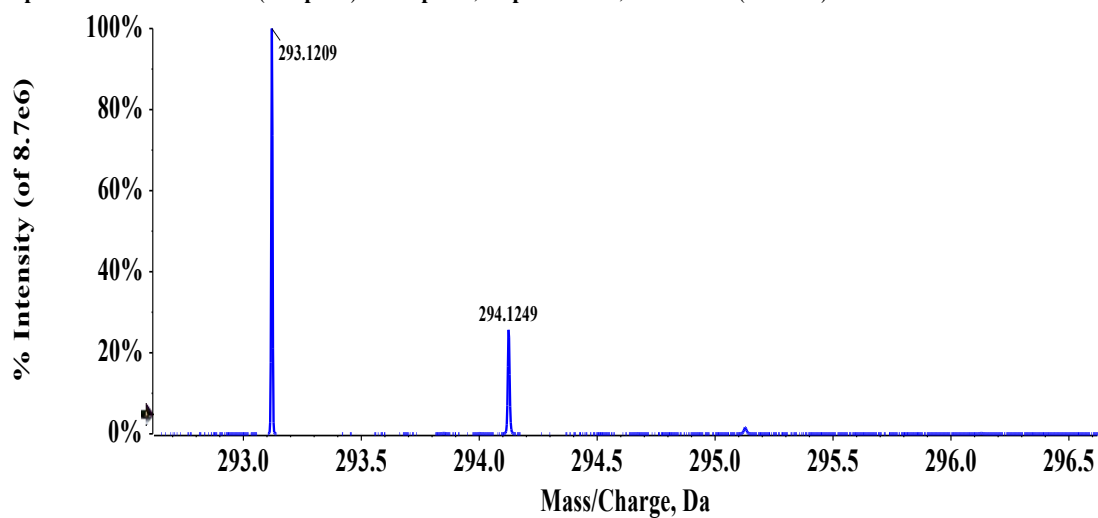


Figure 18. HRMS spectrum of title compound 5e

Compound 5f

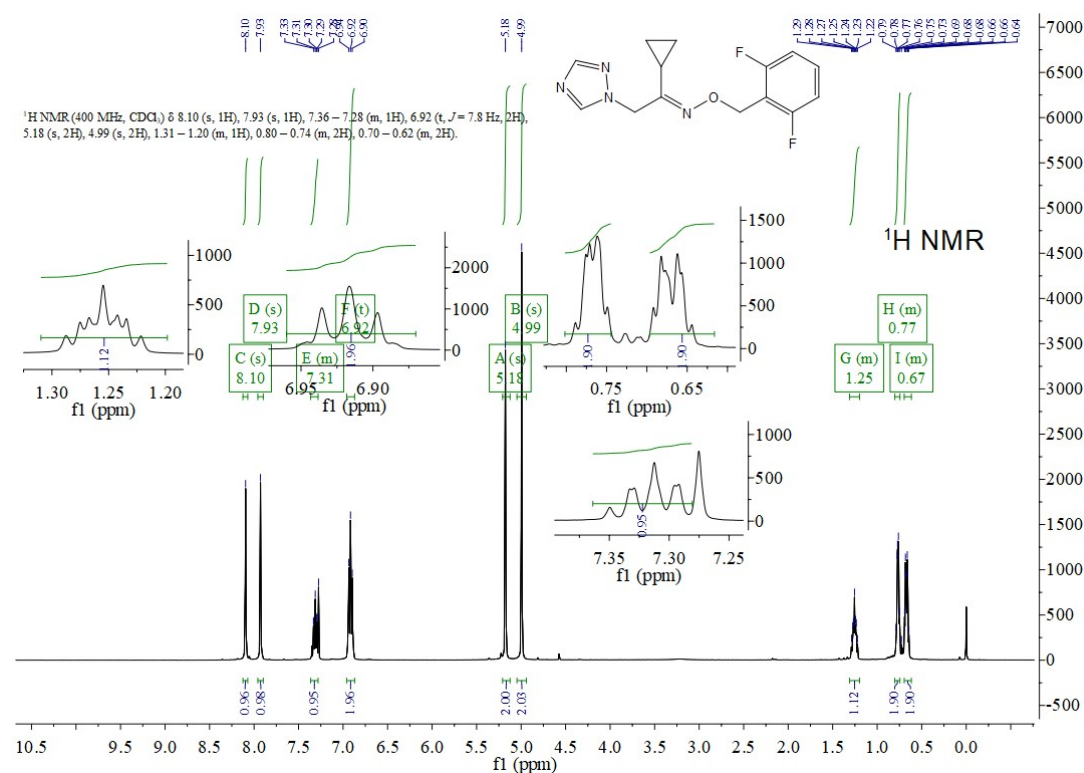


Figure 19. ¹H NMR spectrum of intermediate 5f

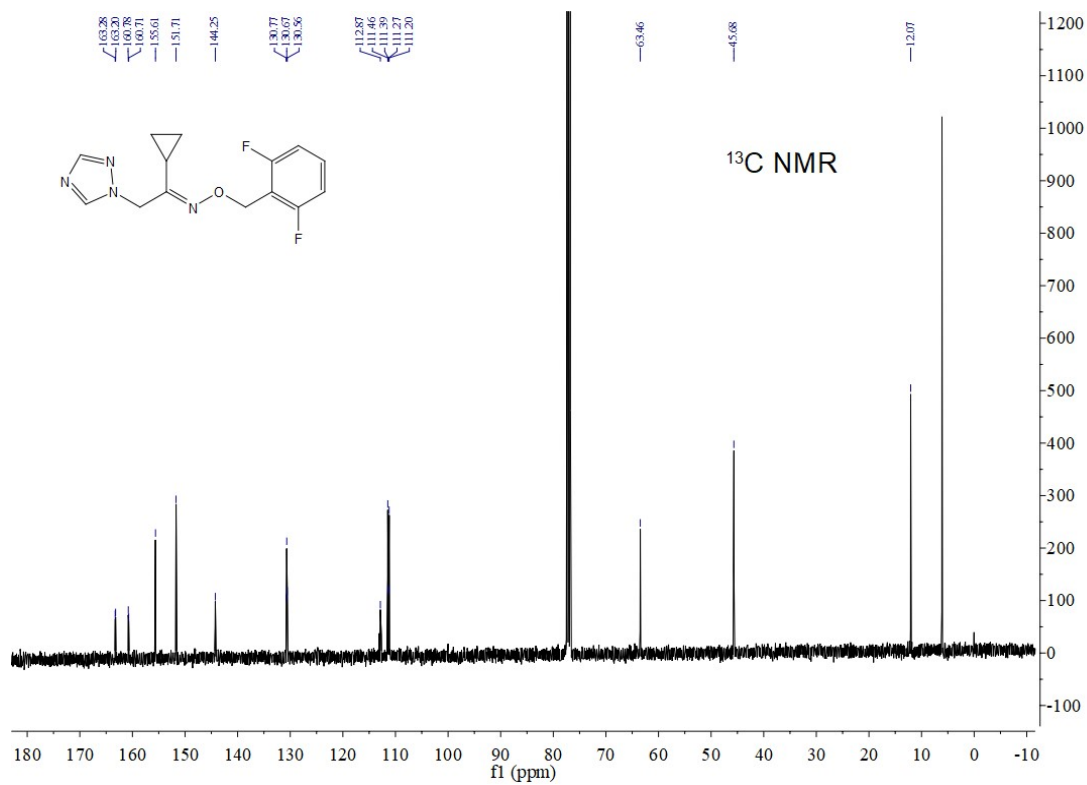


Figure 20. ¹³C NMR spectrum of title compound 5f

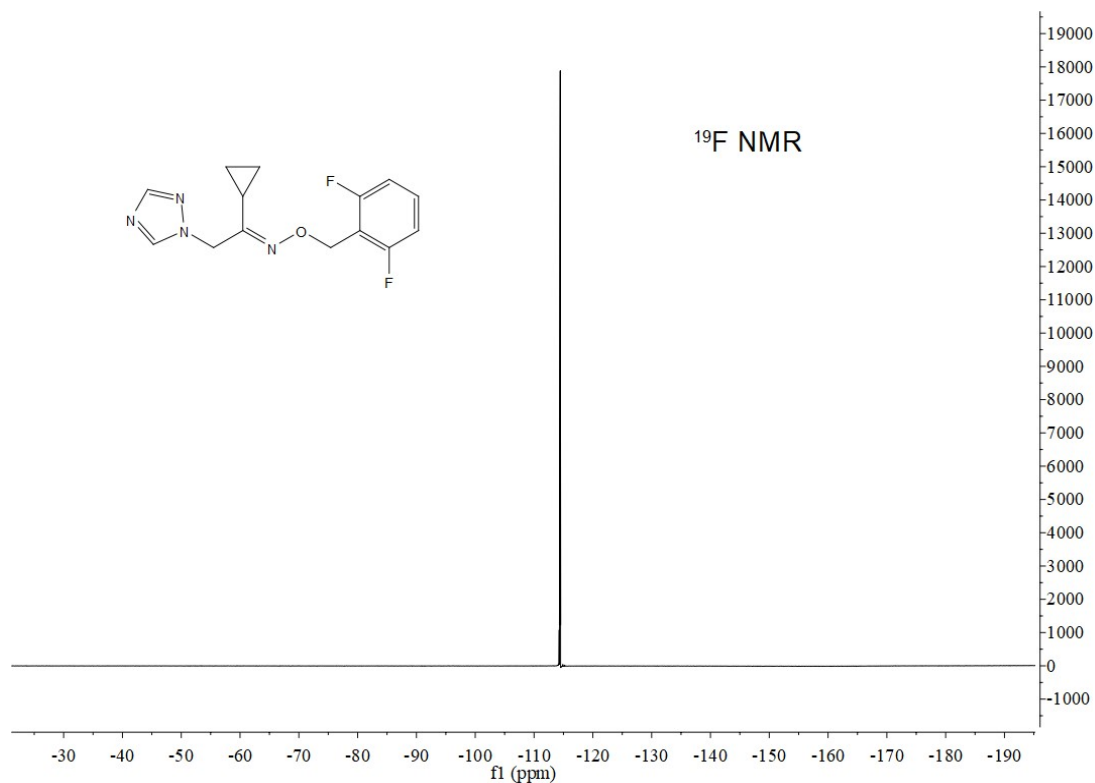


Figure 21. ¹⁹F NMR spectrum of title compound 5f

Spectrum from A06.wiff (sample 1) - Sample06, Experiment 1, +TOF MS (80 - 800) from 0.085 to 0.094 min

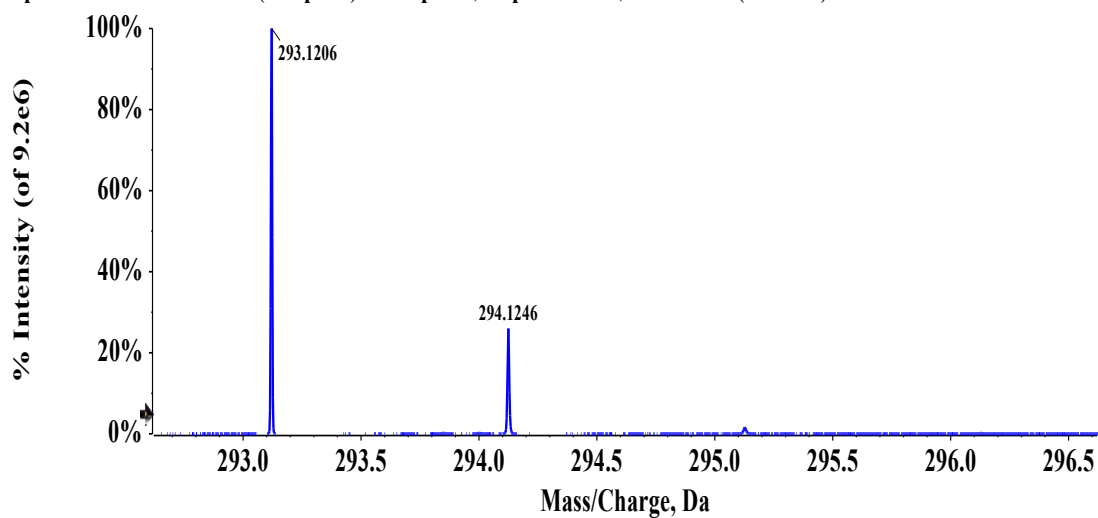


Figure 22. HRMS spectrum of title compound 5f

Compound 5g

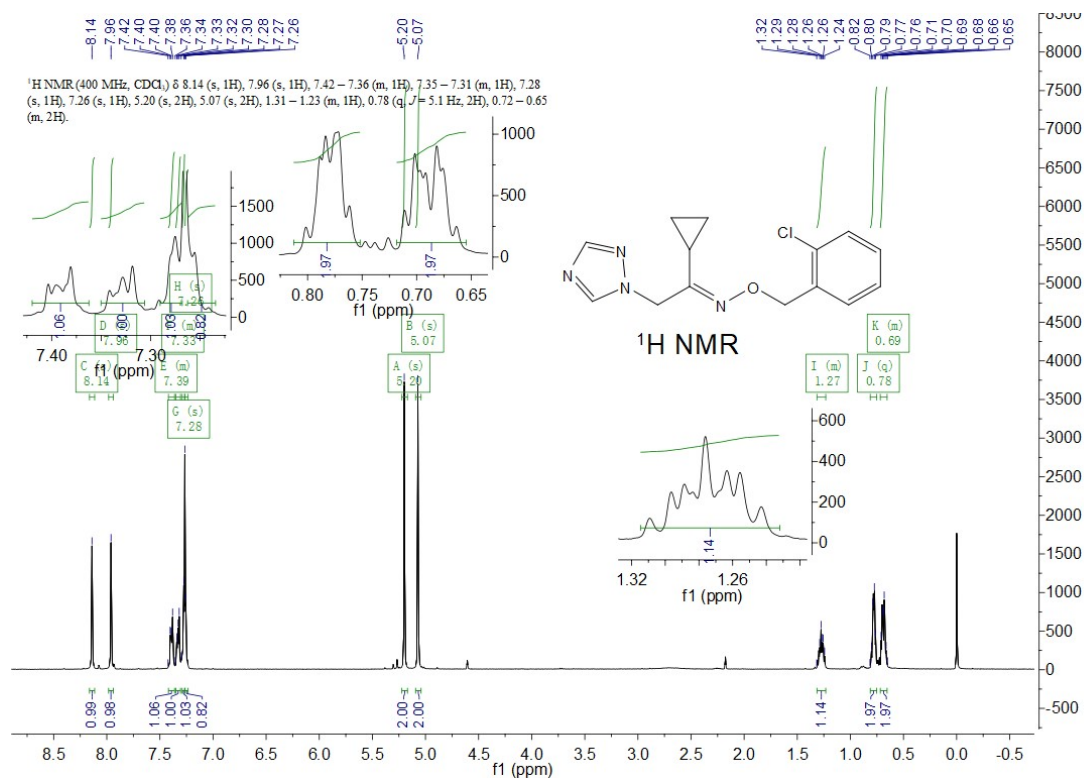


Figure 23. ¹H NMR spectrum of title compound 5g

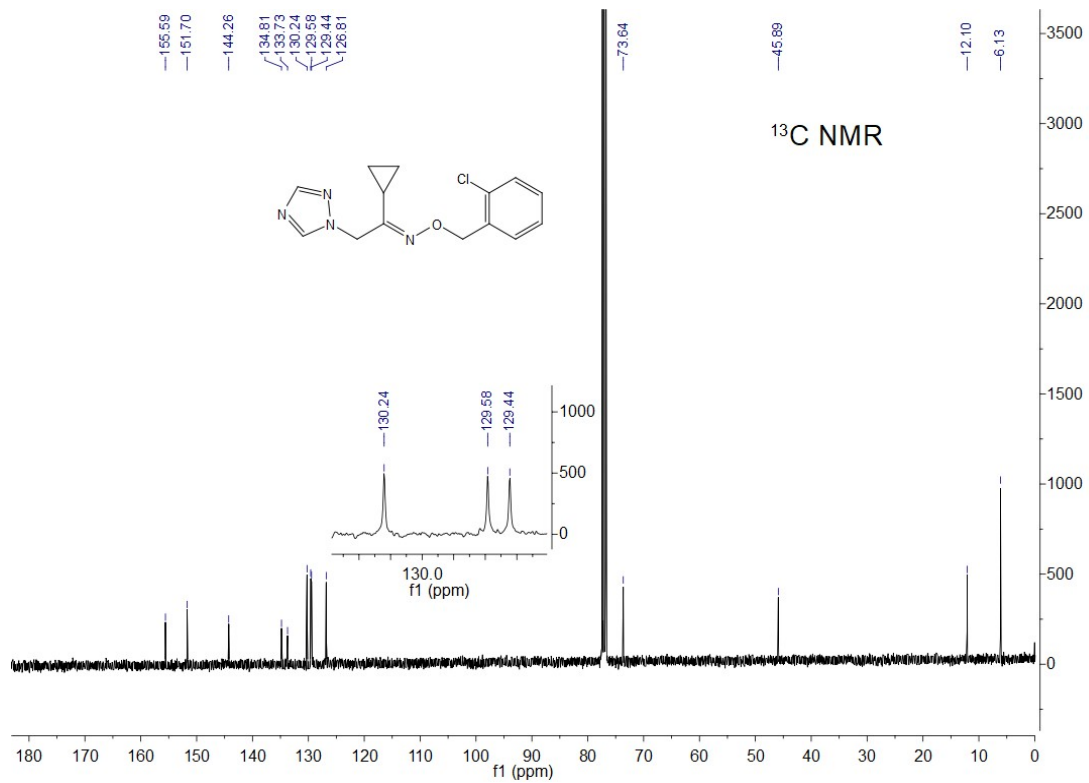


Figure24. ¹³C NMR spectrum of title compound 5g

Spectrum from A07.wiff (sample 1) - Sample07, Experiment 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

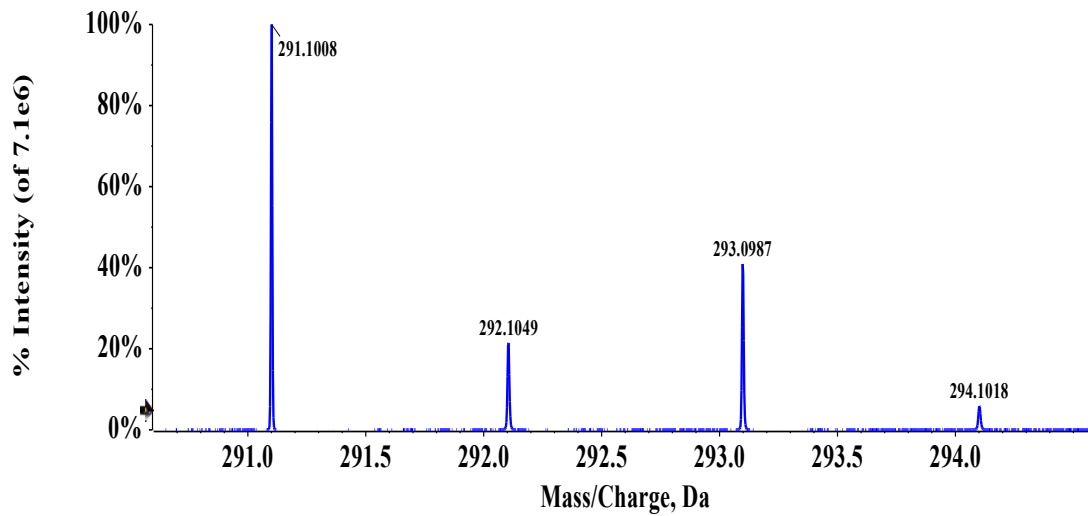


Figure 25. HRMS spectrum of title compound 5g

Compound 5h

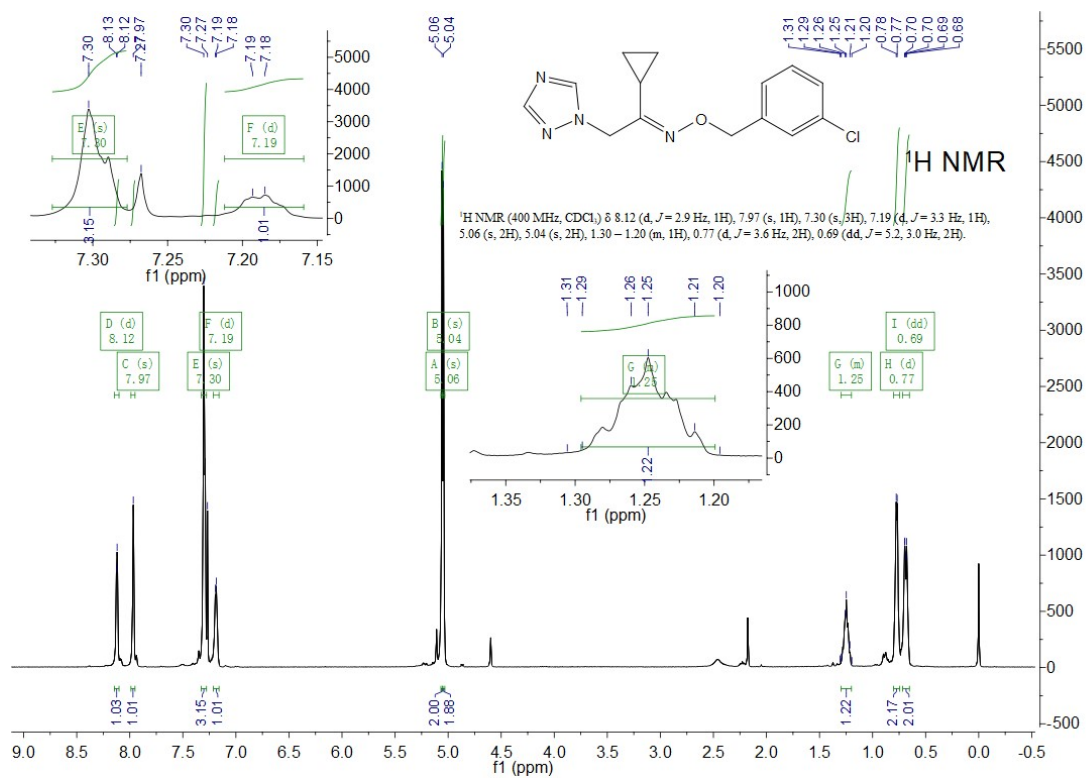


Figure 26. ¹H NMR spectrum of title compound 5h

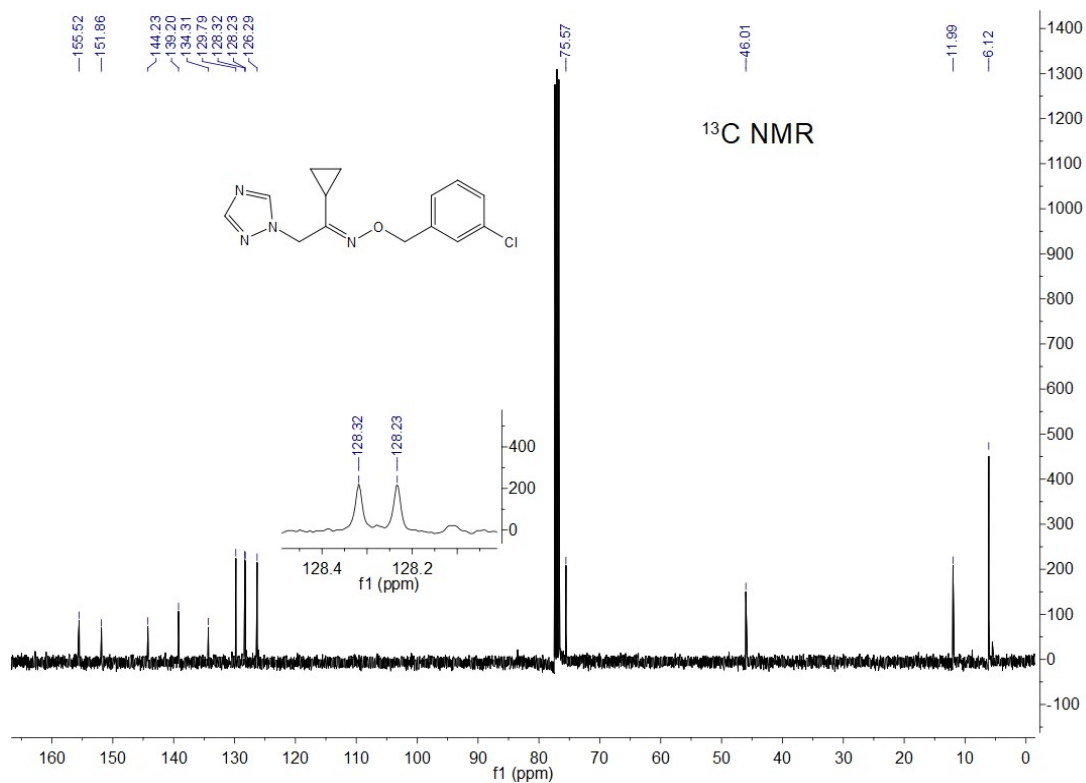


Figure 27. ¹³C NMR spectrum of title compound 5h

Spectrum from A08.wiff (sample 1) - Sample08, Experiment 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

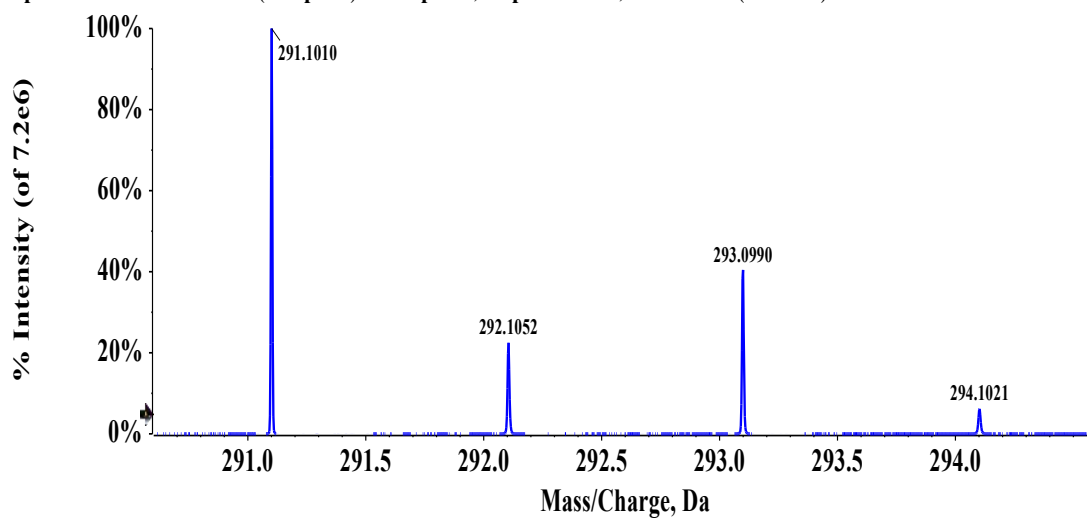


Figure 28. HRMS spectrum of title compound 5h

Compound 5i

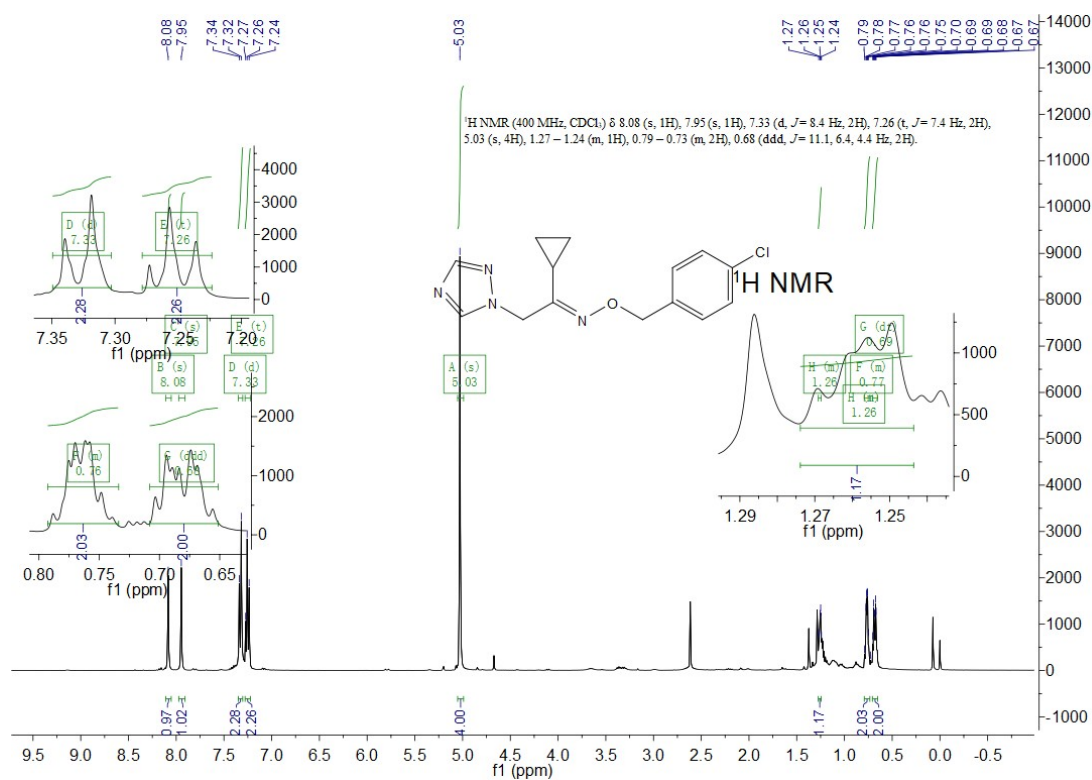


Figure 29. ¹H NMR spectrum of title compound 5i

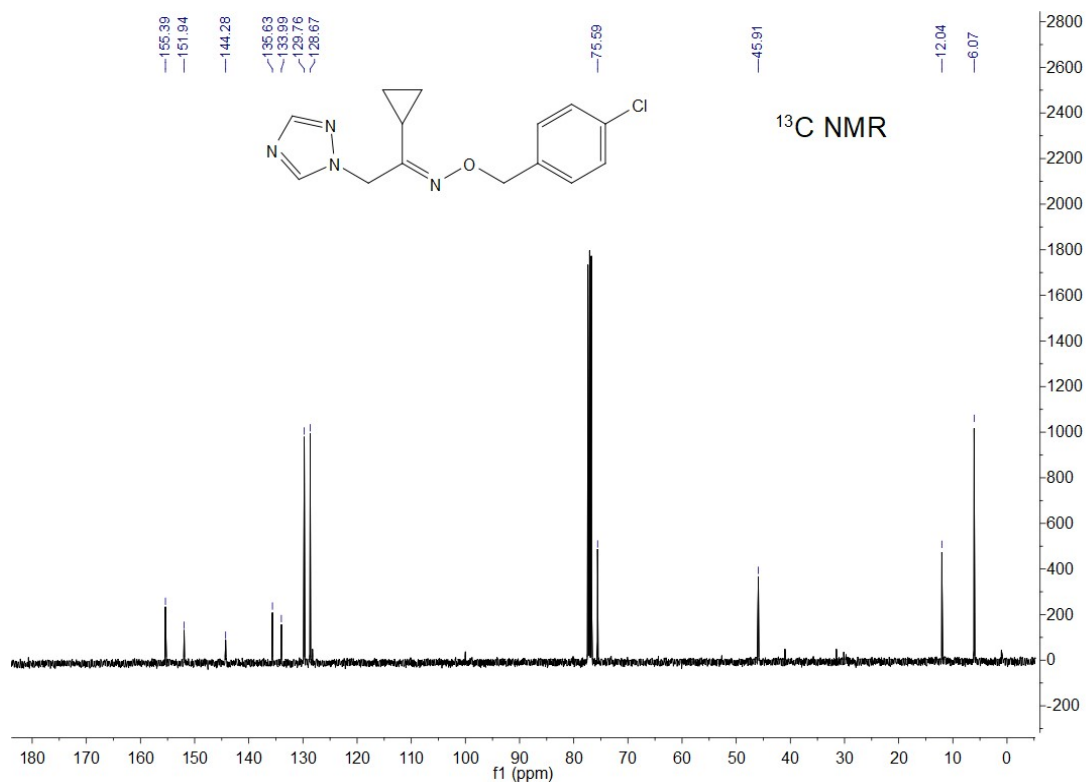


Figure 30. ¹³C NMR spectrum of title compound 5i

Spectrum from A09.wiff (sample 1) - Sample09, Experiment 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

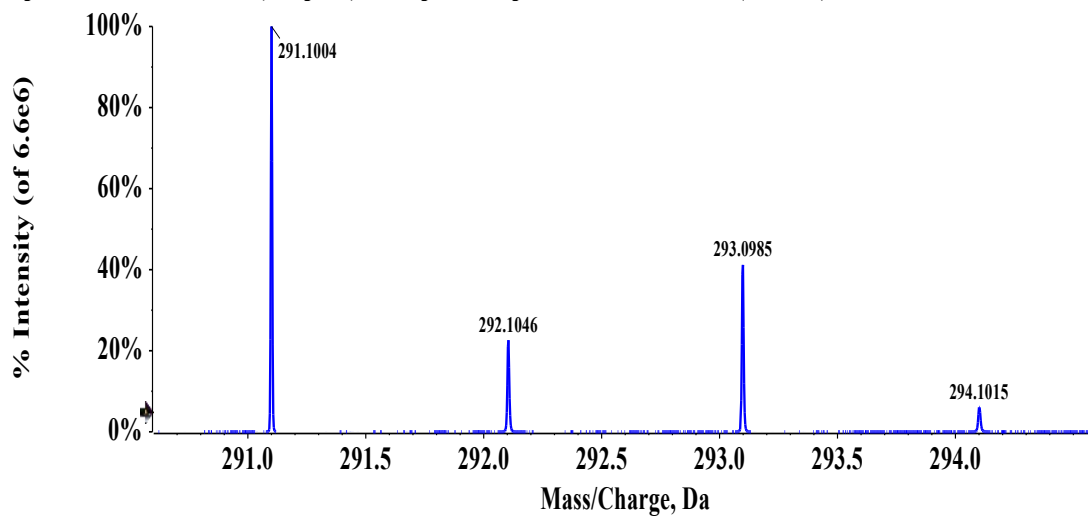


Figure 31. HRMS spectrum of title compound 5i

Compound 5j

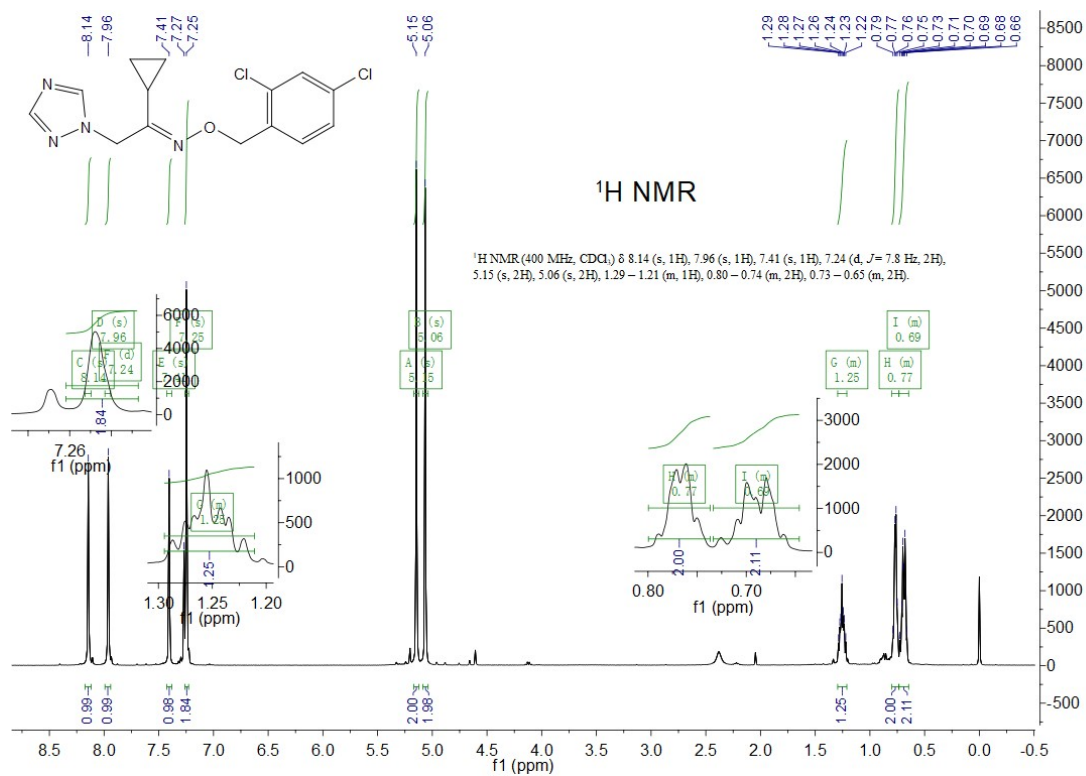


Figure 32. ¹H NMR spectrum of title compound 5j

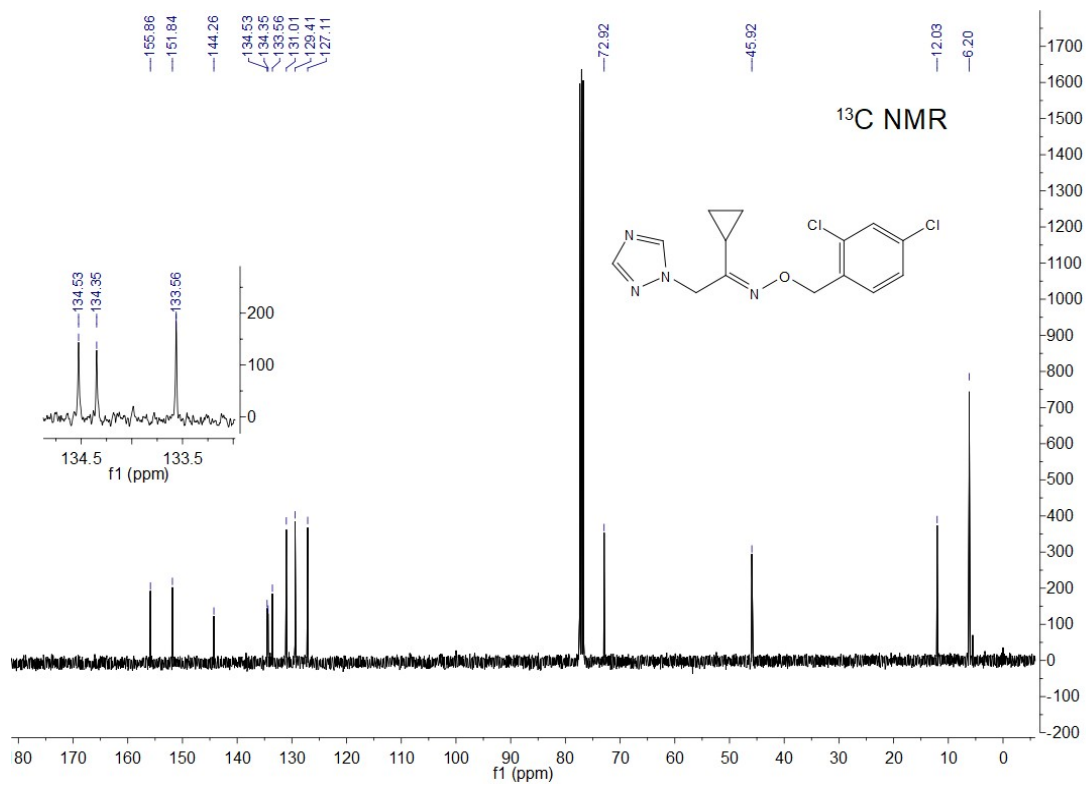


Figure 33. ¹³C NMR spectrum of title compound 5j

Spectrum from A10.wiff (sample 1) - Sample10, Experiment 1, +TOF MS (80 - 800) from 0.082 to 0.091 min

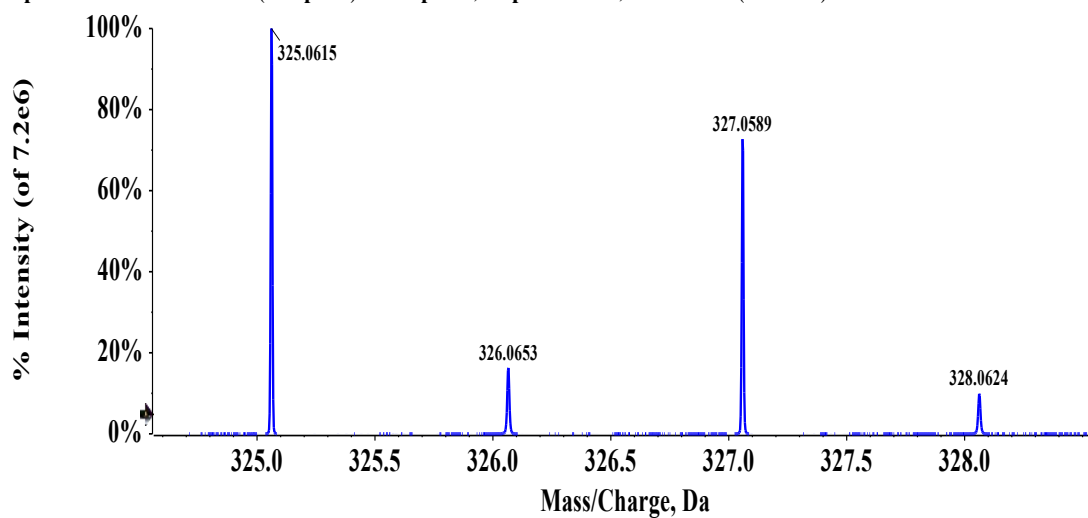


Figure 34. HRMS spectrum of title compound 5j

Compound 5k

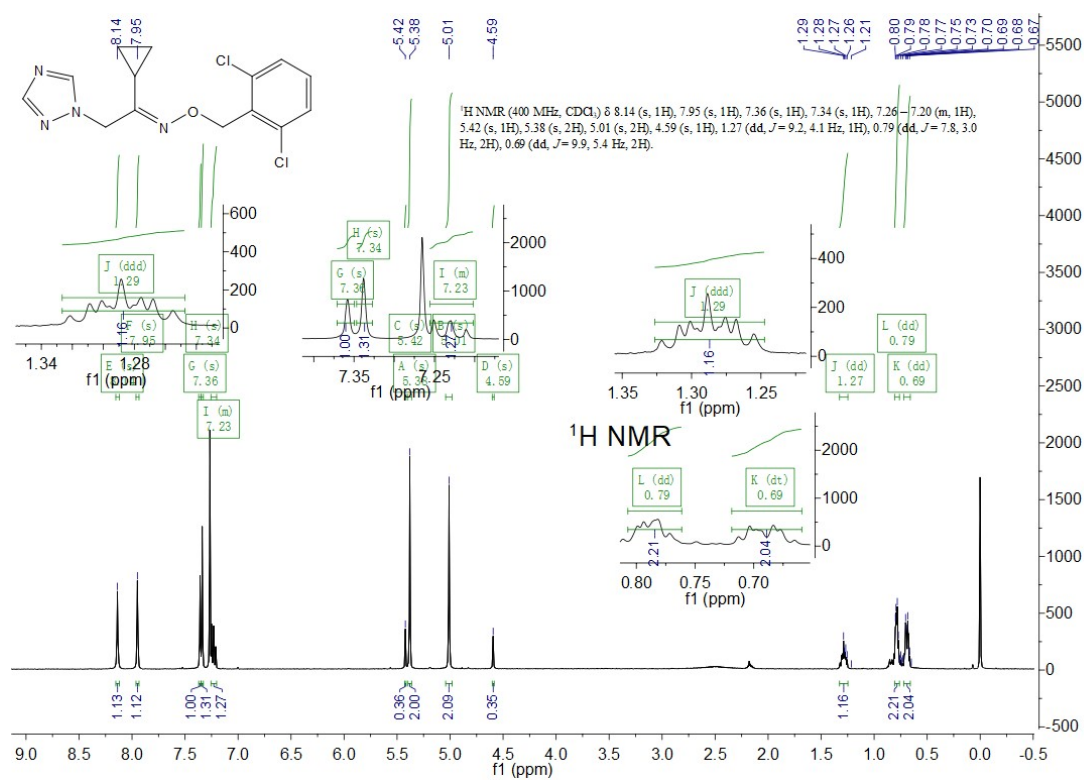


Figure 35. ¹H NMR spectrum of title compound 5k

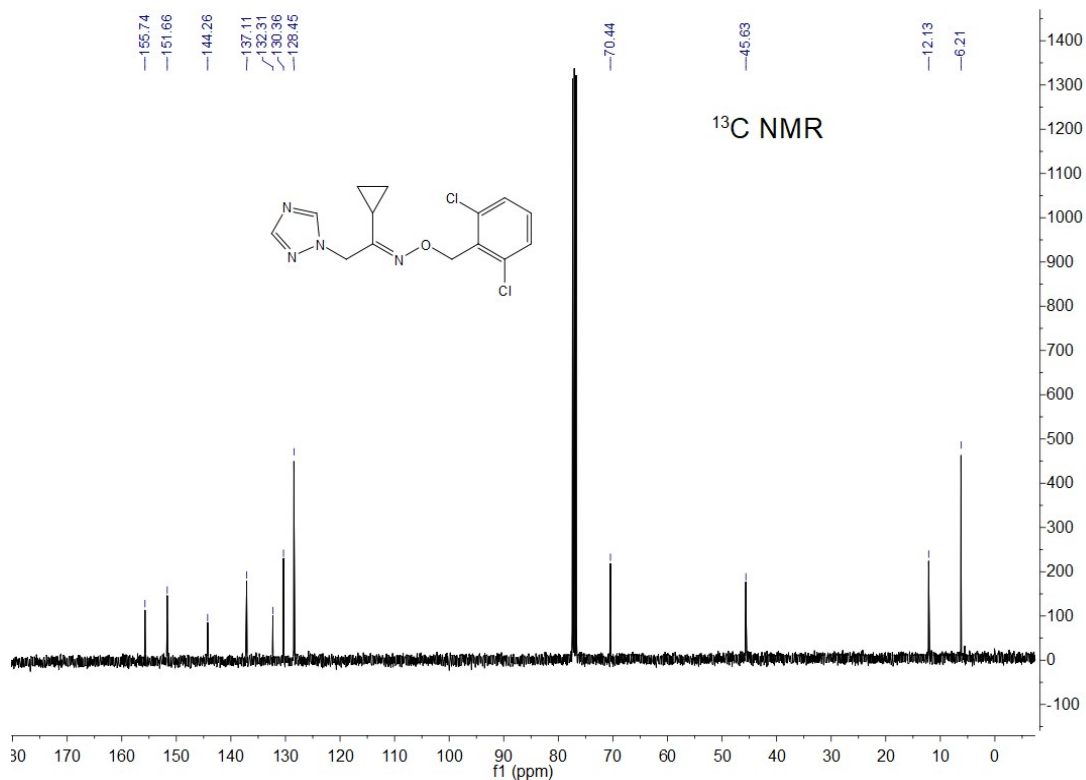


Figure 36. ¹³C NMR spectrum of title compound 5k

Spectrum from A11.wiff (sample 1) - Sample11, Experiment 1, +TOF MS (80 - 800) from 0.067 to 0.076 min

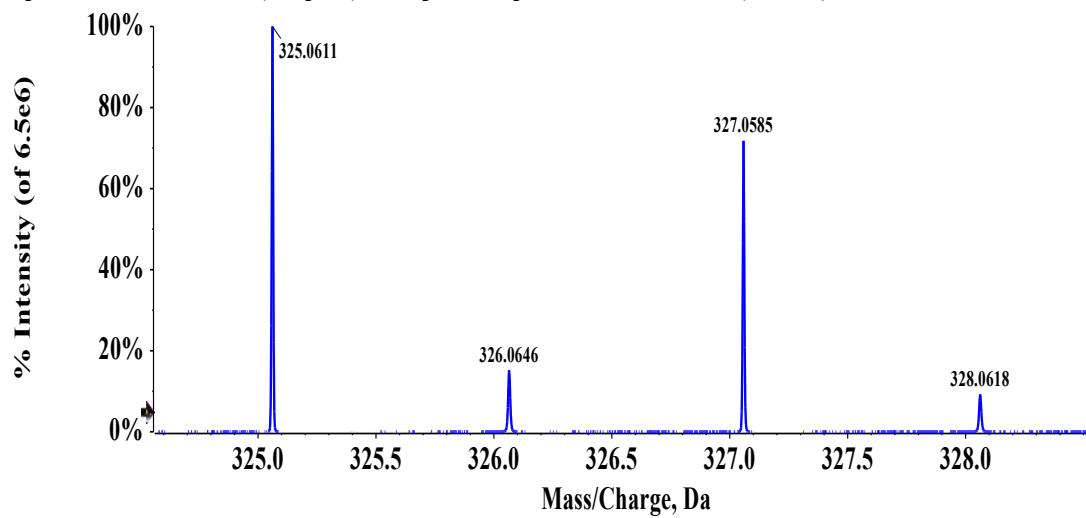


Figure 37. HRMS spectrum of title compound 5k

Compound 51

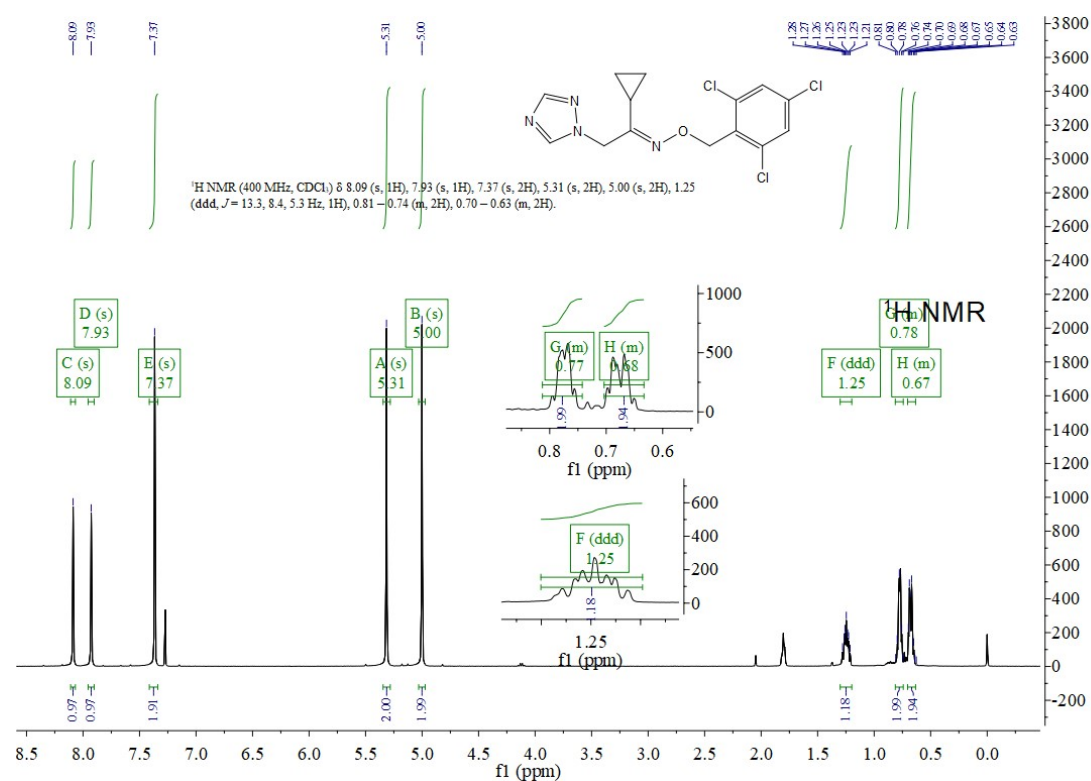


Figure 38. ¹H NMR spectrum of title compound 51

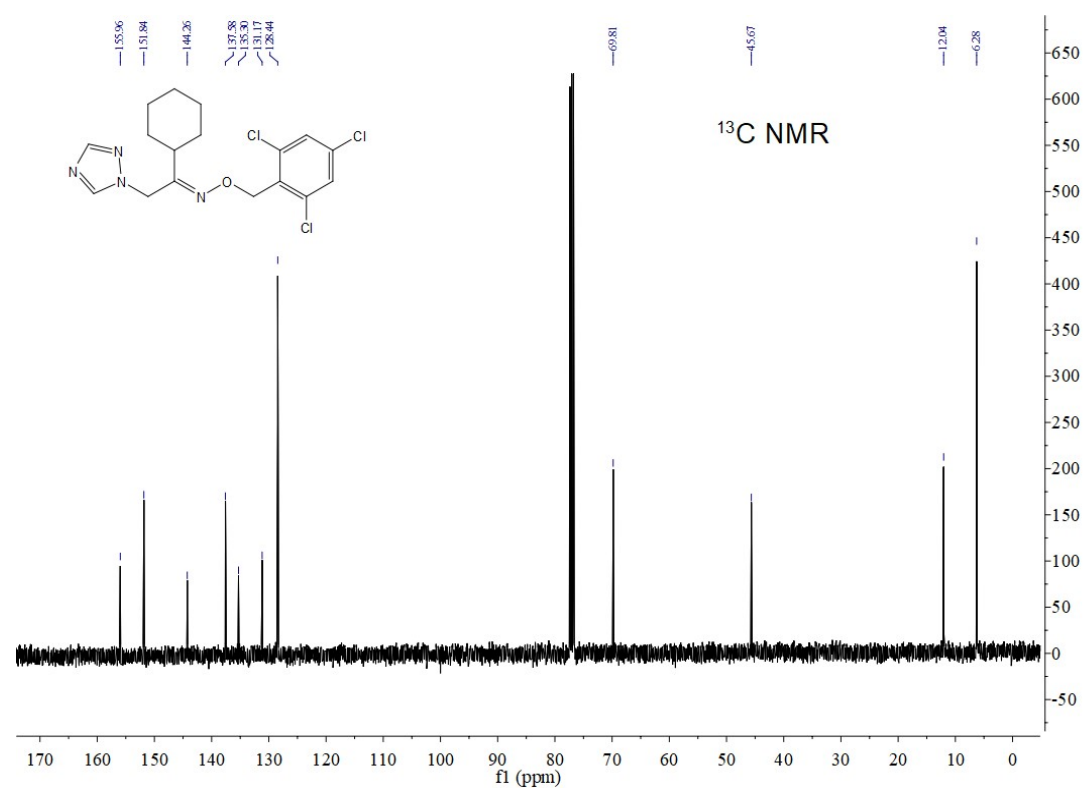


Figure 39. ¹³C NMR spectrum of title compound 51

Spectrum from B12.wiff (sample 1) - B12, Experiment 1, +TOF MS (80 - 800) from 0.064 to 0.073 min

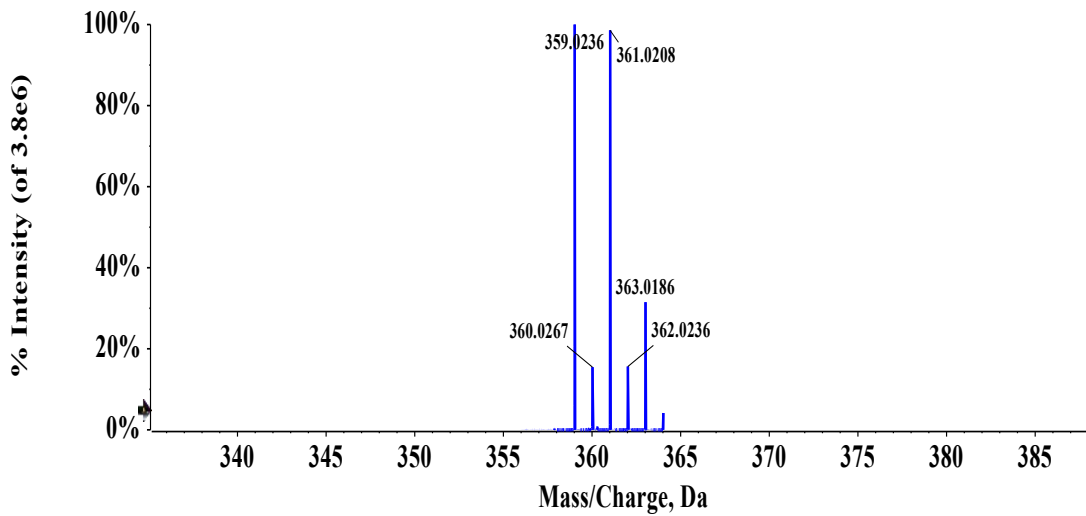


Figure 40. HRMS spectrum of title compound 5l

Compound 5m

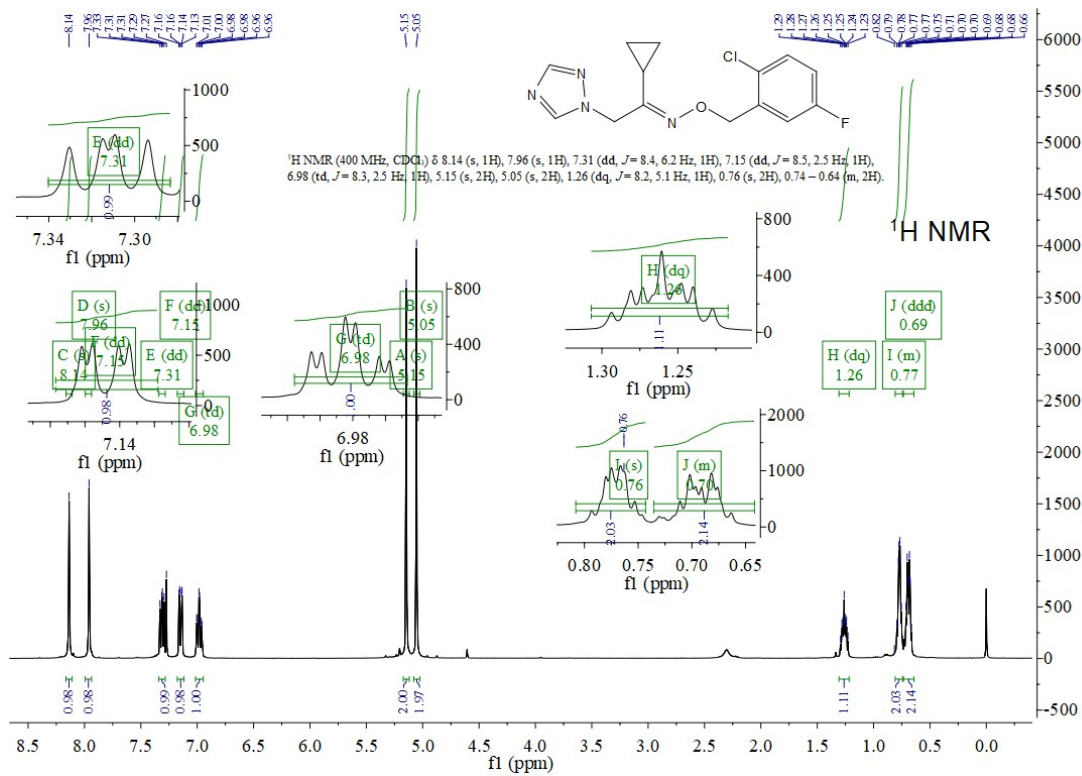


Figure 41. ¹H NMR spectrum of title compound 5m

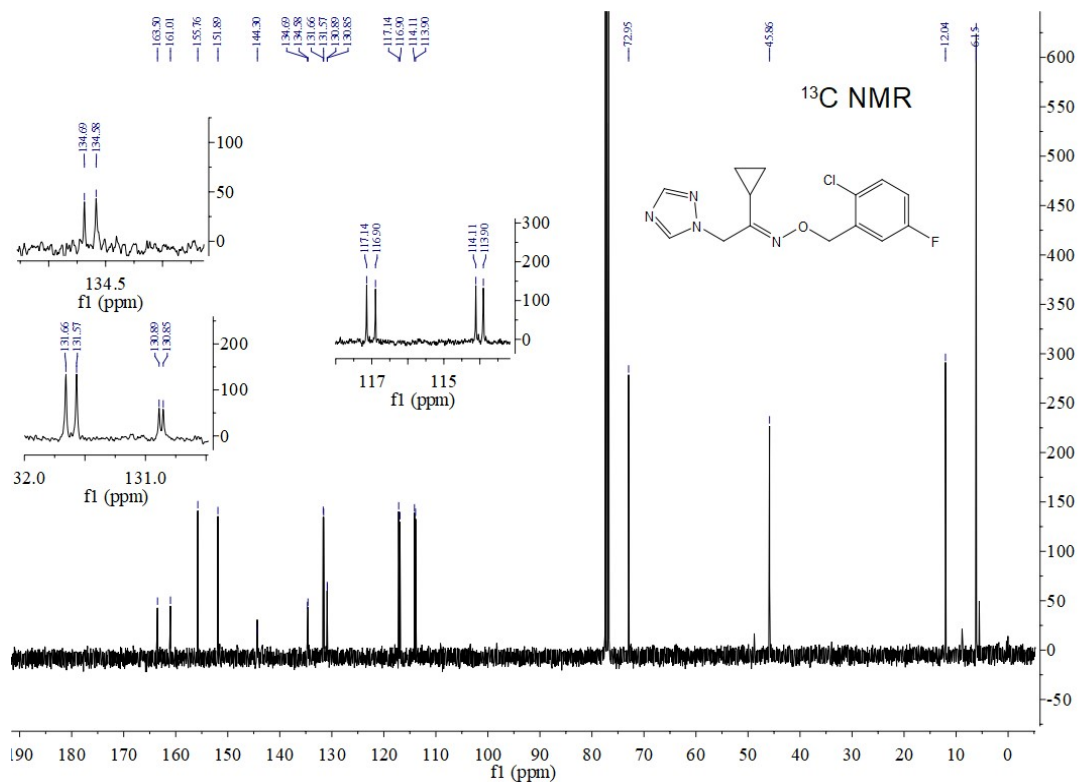


Figure 42. ¹³C NMR spectrum of title compound 5m

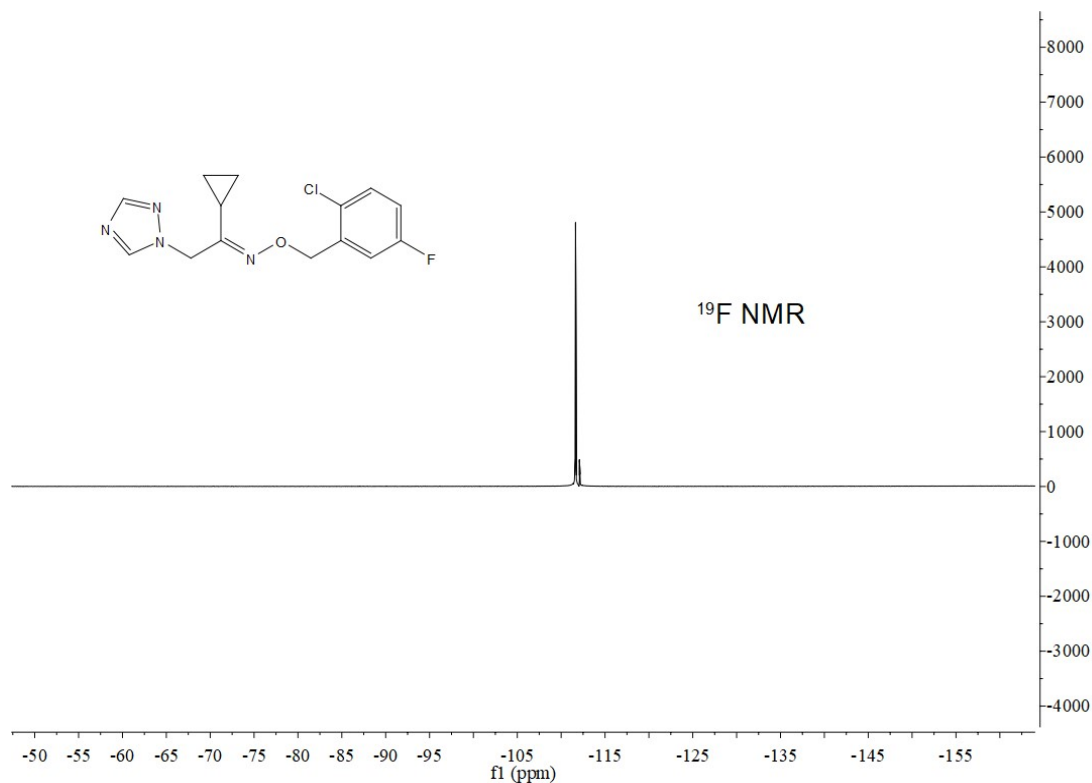


Figure 43. ¹⁹F NMR spectrum of title compound 5m

Spectrum from A12.wiff (sample 1) - Sample12, Experiment 1, +TOF MS (80 - 800) from 0.073 to 0.082 min

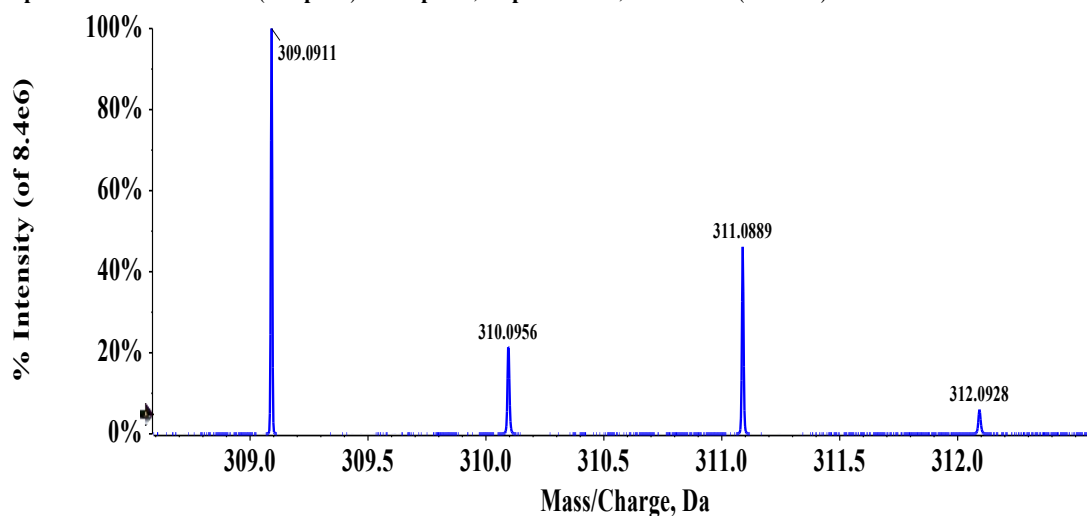


Figure 44. HRMS spectrum of title compound 5m

Compound 5n

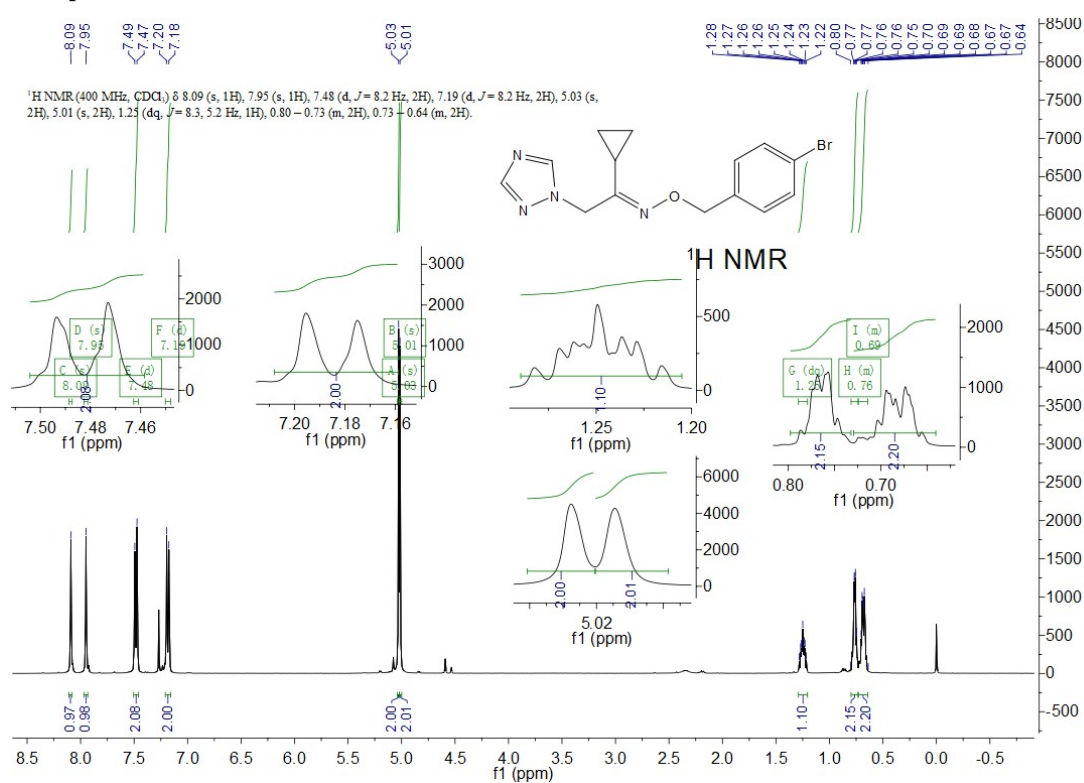


Figure 45. ¹H NMR spectrum of title compound 5n

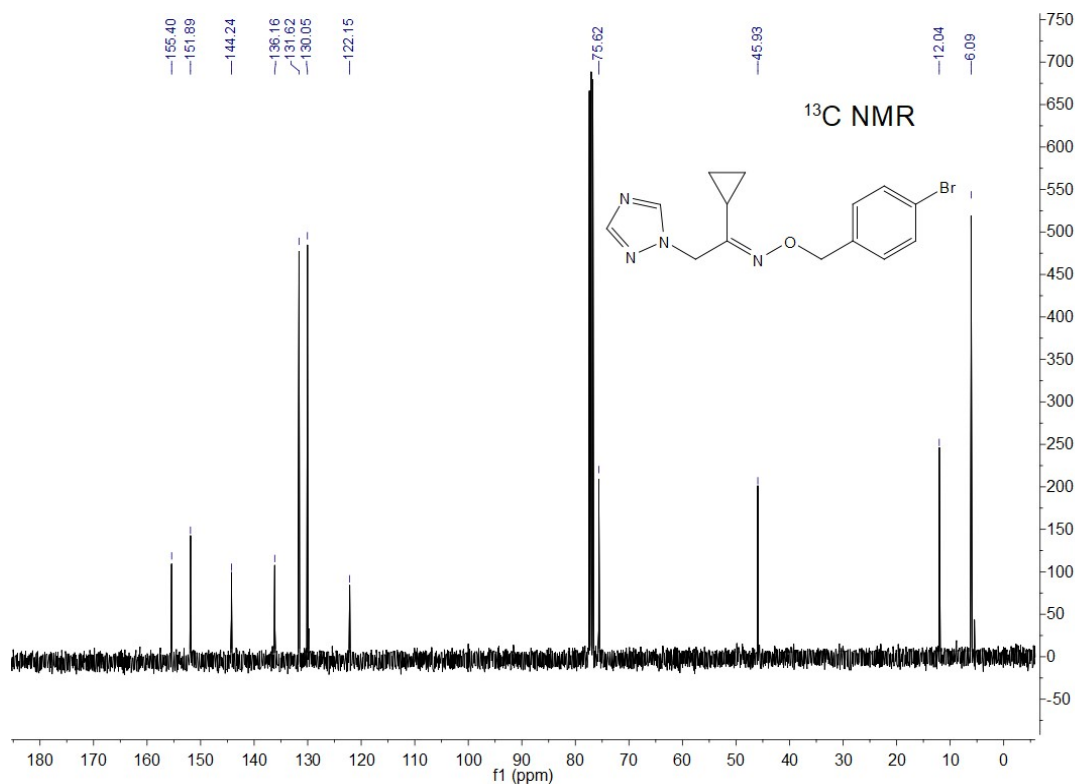


Figure 46. ¹³C NMR spectrum of title compound 5n

Spectrum from A13.wiff (sample 1) - Sample13, Experiment 1, +TOF MS (80 - 800) from 0.076 to 0.085 min

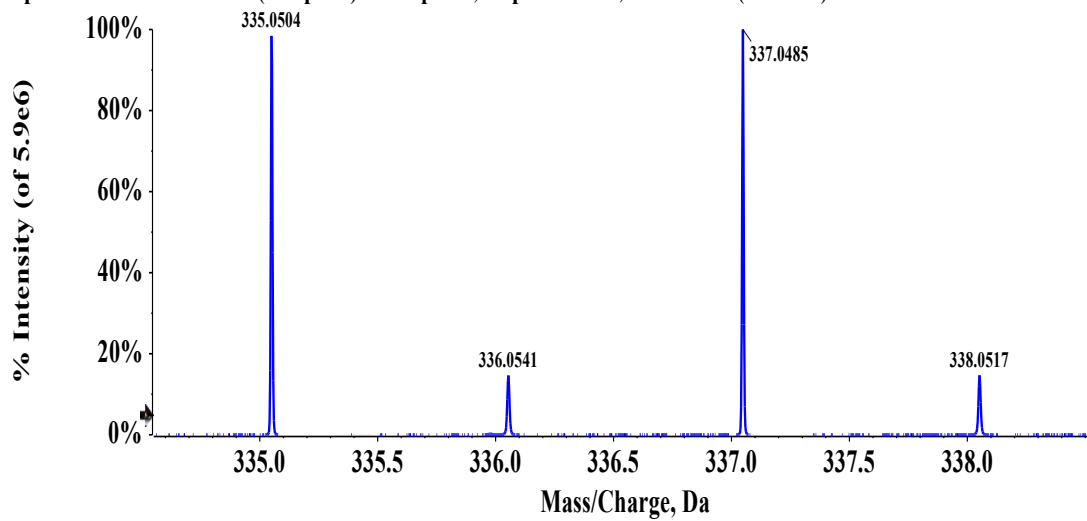


Figure 47. HRMS spectrum of title compound 5n

Compound 5o

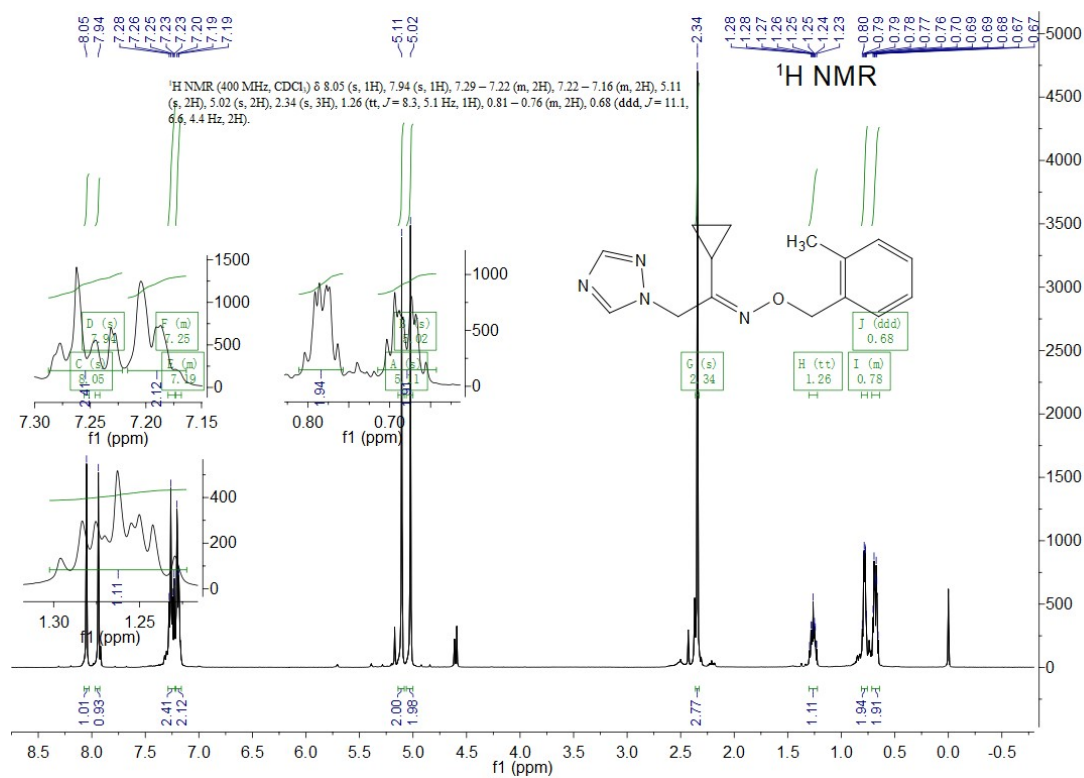


Figure 48. ¹H NMR spectrum of title compound 5o

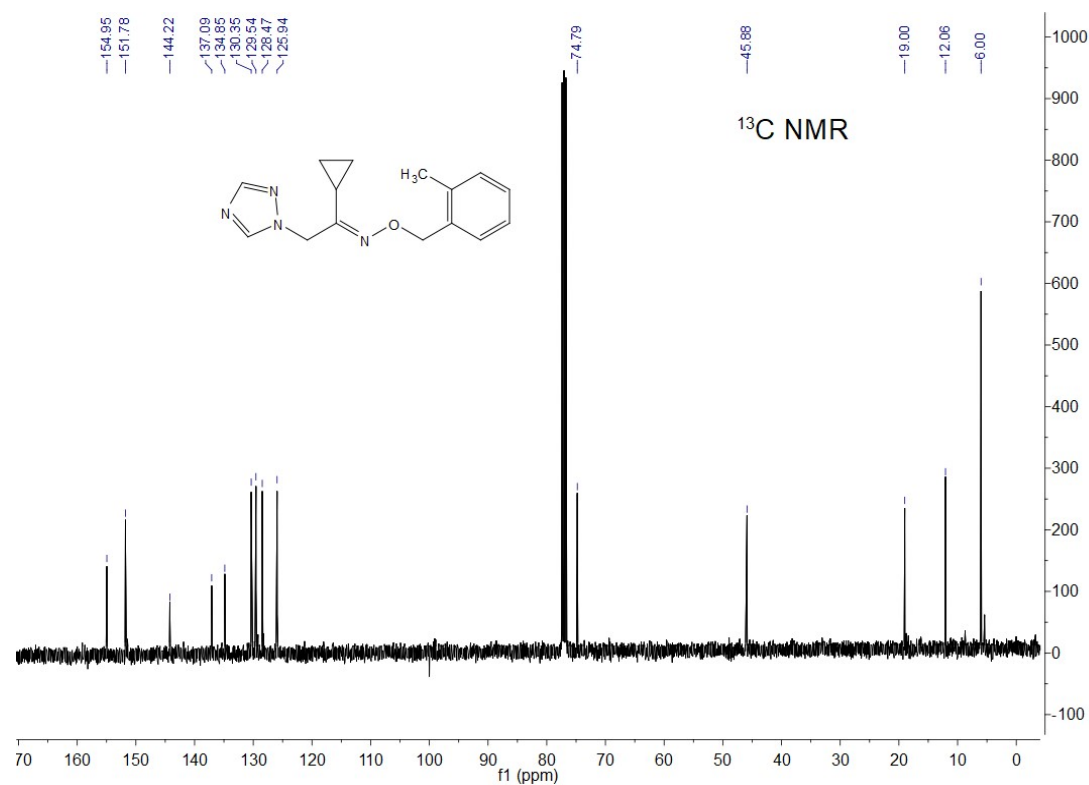


Figure 49. ¹³C NMR spectrum of title compound 5o

Spectrum from A14.wiff (sample 1) - Sample14, Experiment 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

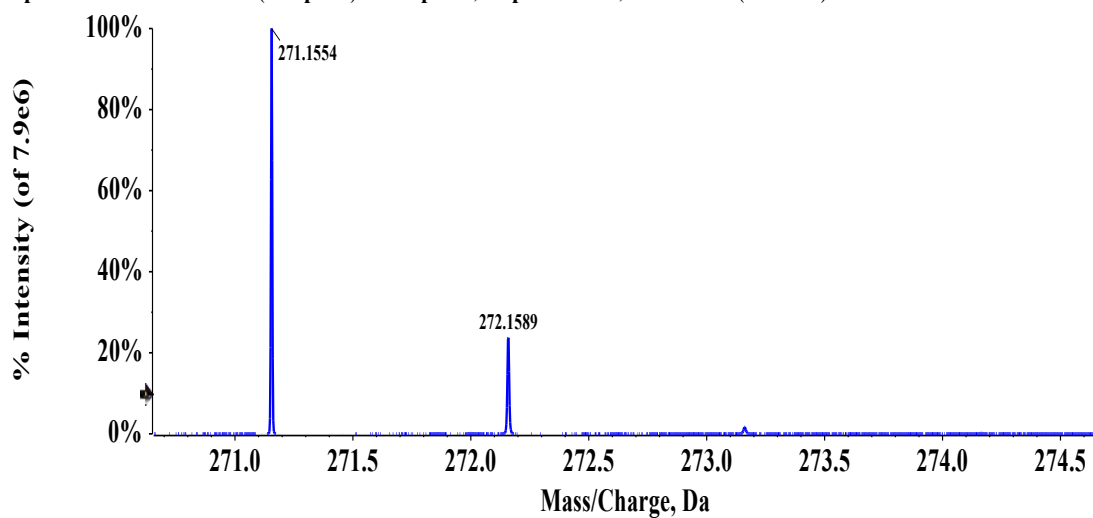


Figure 50. HRMS spectrum of title compound 5o

Compound 5p

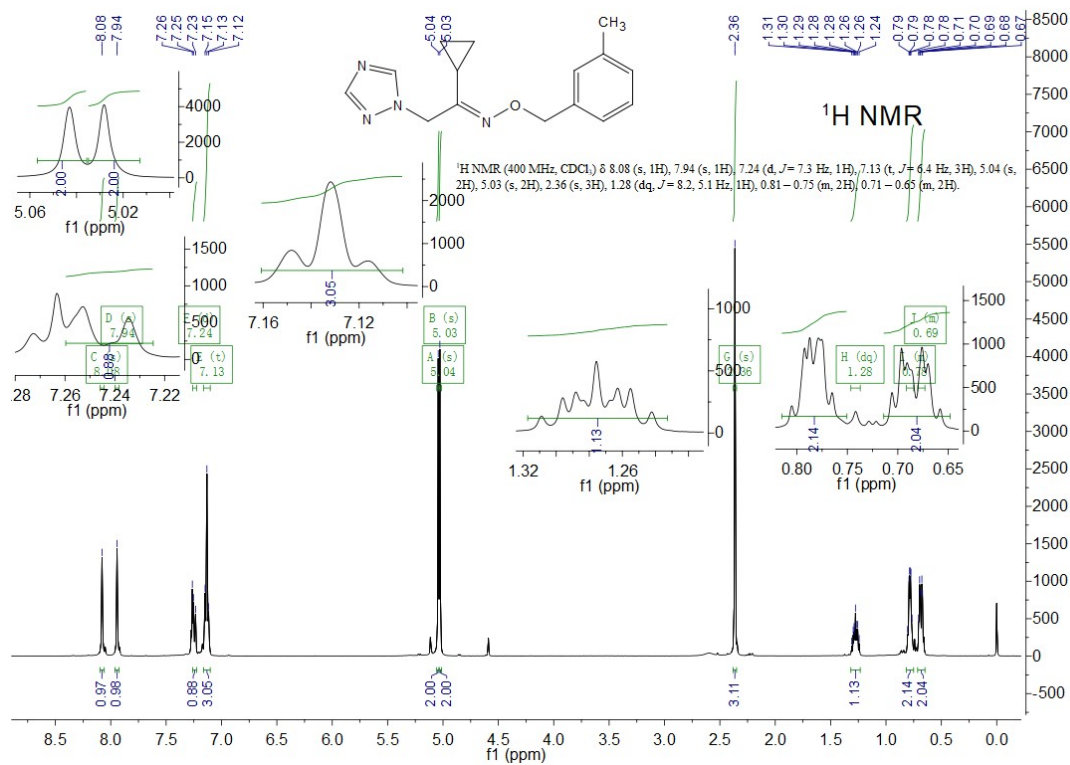


Figure 51. ¹H NMR spectrum of title compound 5p

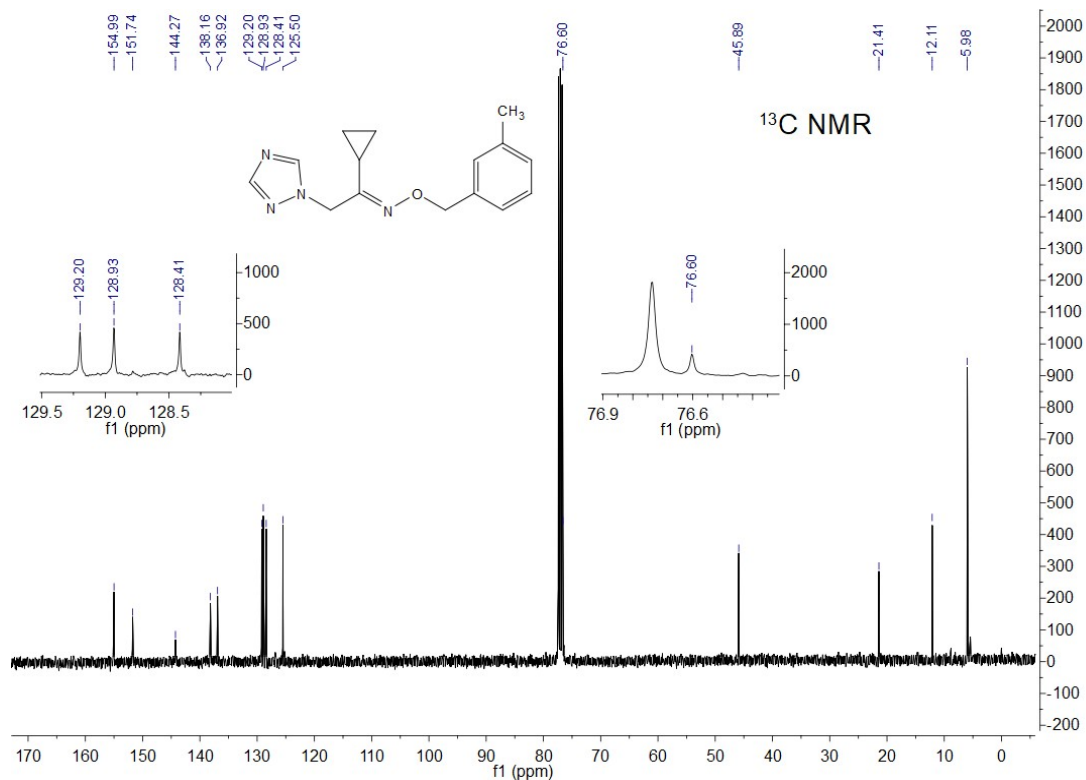


Figure 52. ¹³C NMR spectrum of title compound 5p

Spectrum from A14.wiff (sample 1) - Sample14, Experiment 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

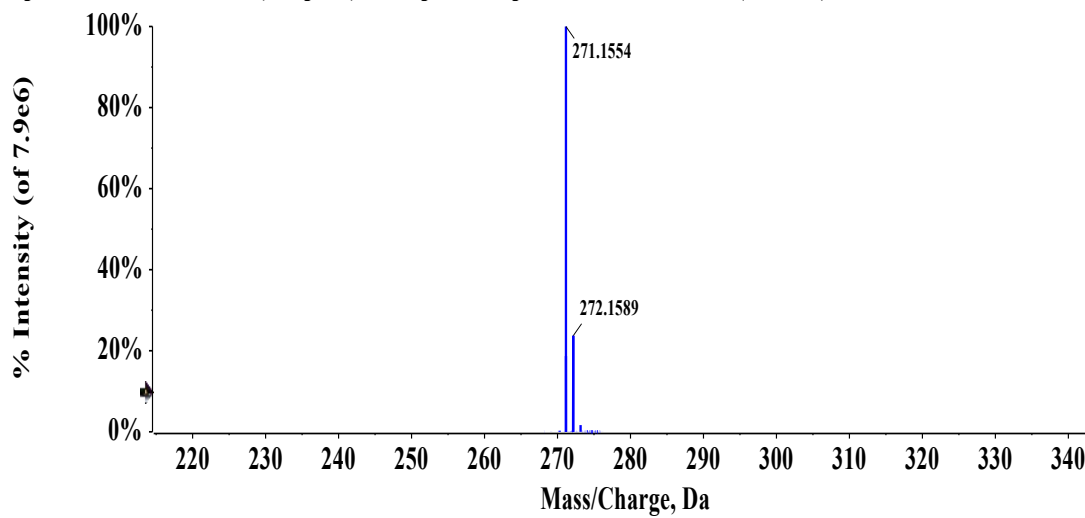


Figure 53. HRMS spectrum of title compound 5p

Compound 5q

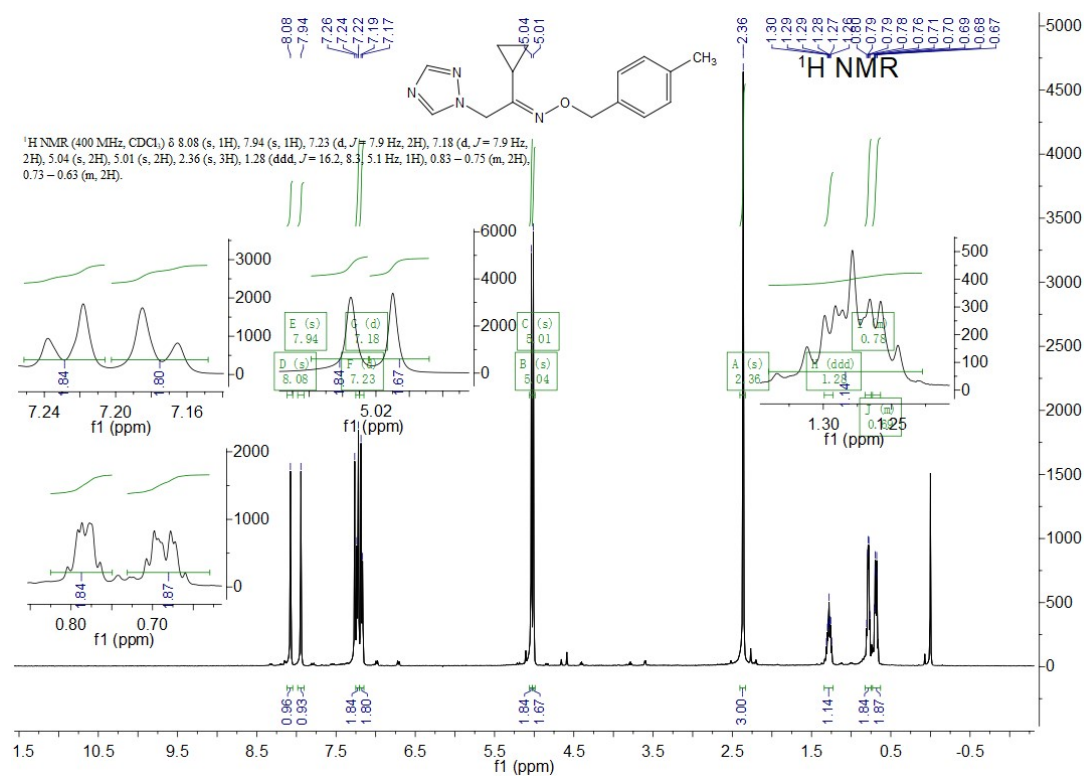


Figure 54. ¹H NMR spectrum of title compound 5q

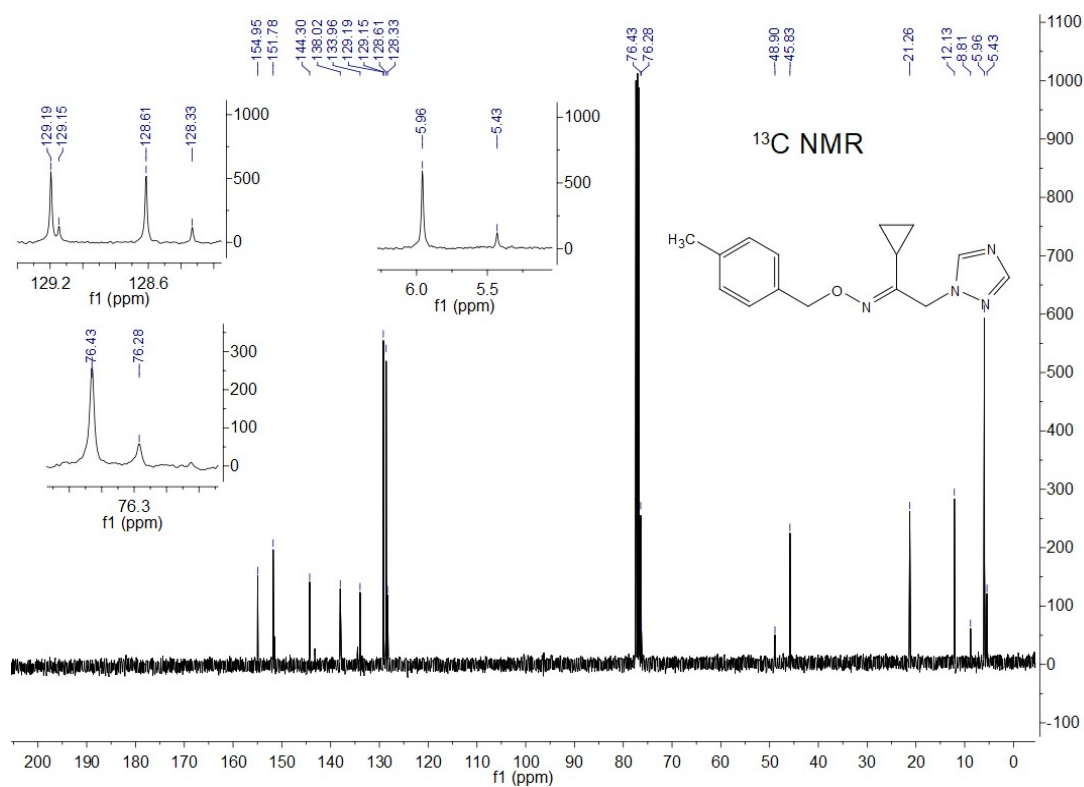


Figure 55. ¹³C NMR spectrum of title compound 5q

Spectrum from A16.wiff (sample 1) - Sample16, Experiment 1, +TOF MS (80 - 800) from 0.091 to 0.108 min

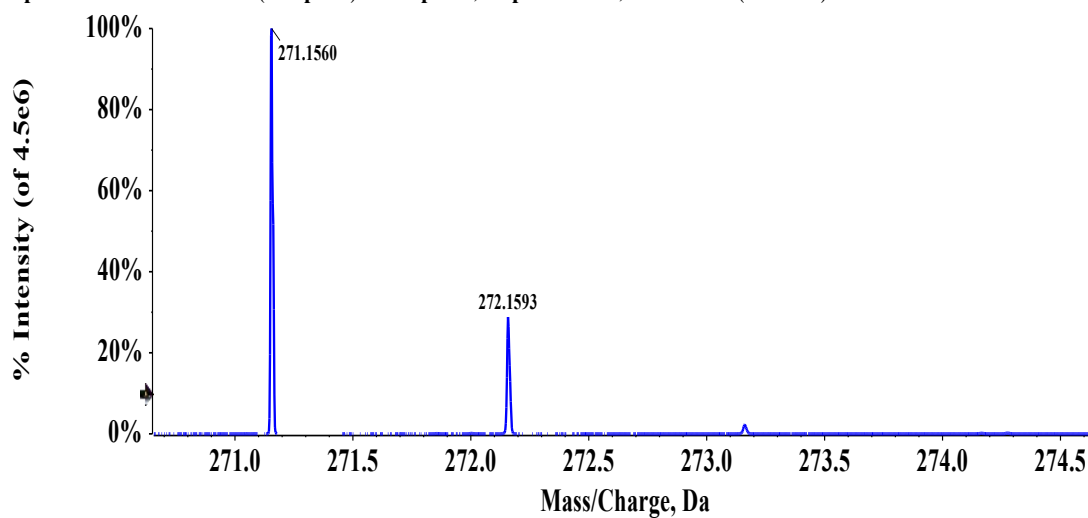


Figure 56. HRMS spectrum of title compound 5q

Compound 5r

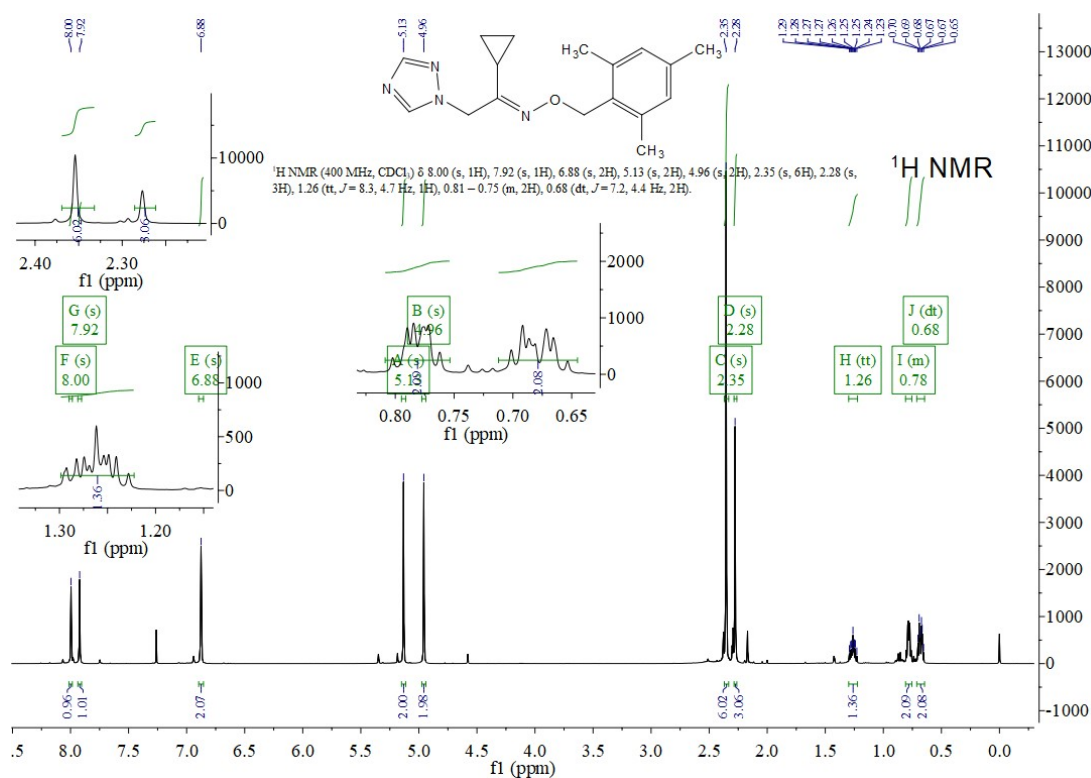


Figure 57. ¹H NMR spectrum of title compound 5r

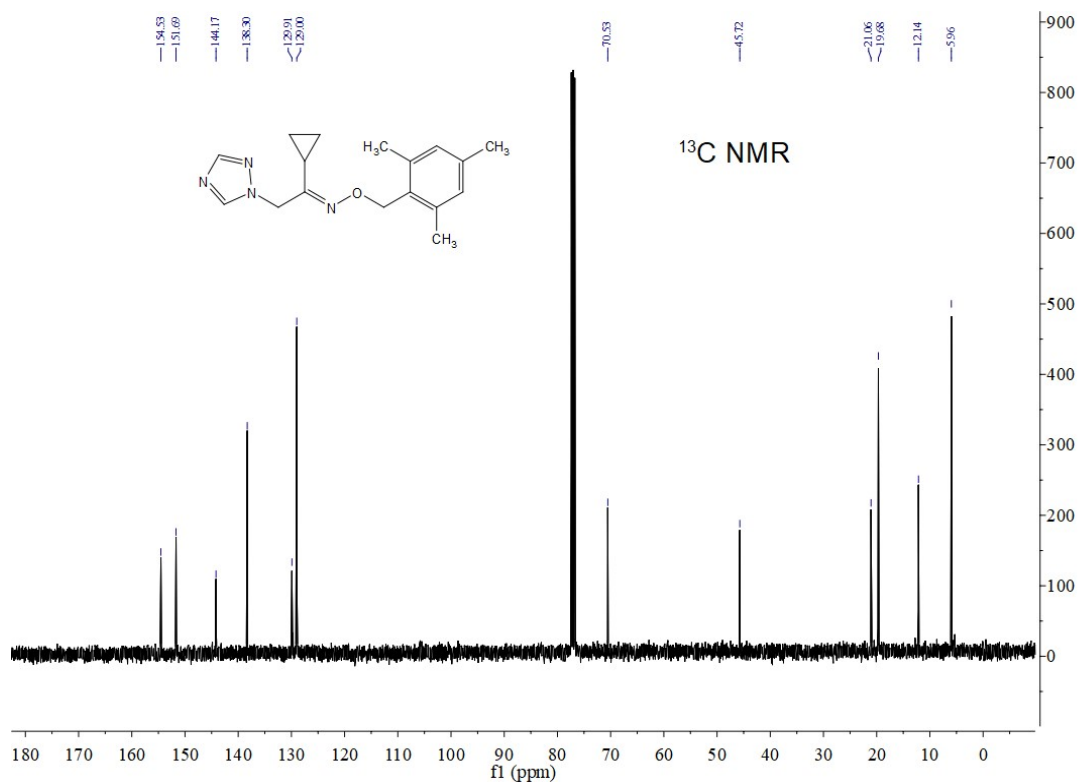


Figure 58. ¹³C NMR spectrum of title compound 5r

Spectrum from A17.wiff (sample 1) - Sample17, Experiment 1, +TOF MS (80 - 800) from 0.090 to 0.107 min

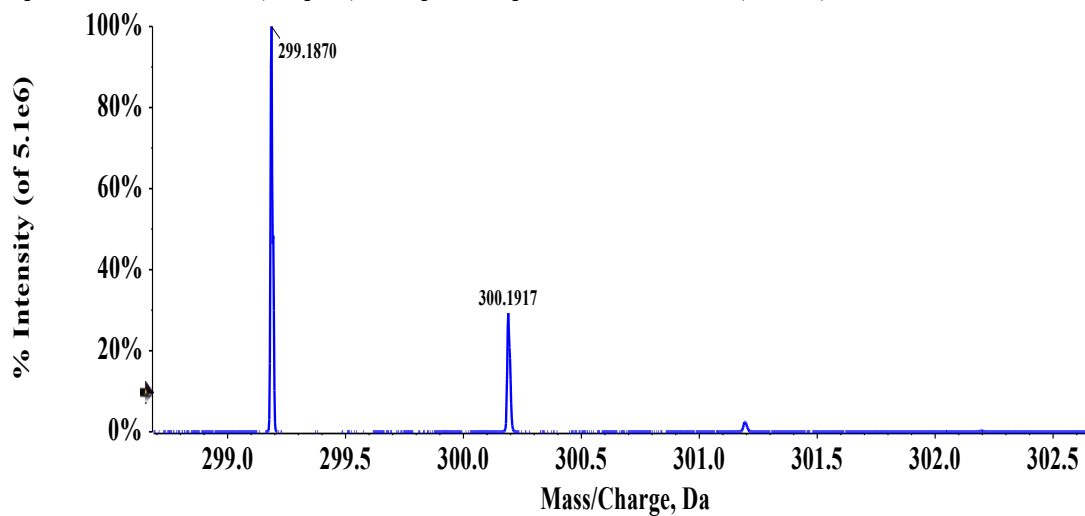


Figure 59. HRMS spectrum of title compound 5r

Compound 5s

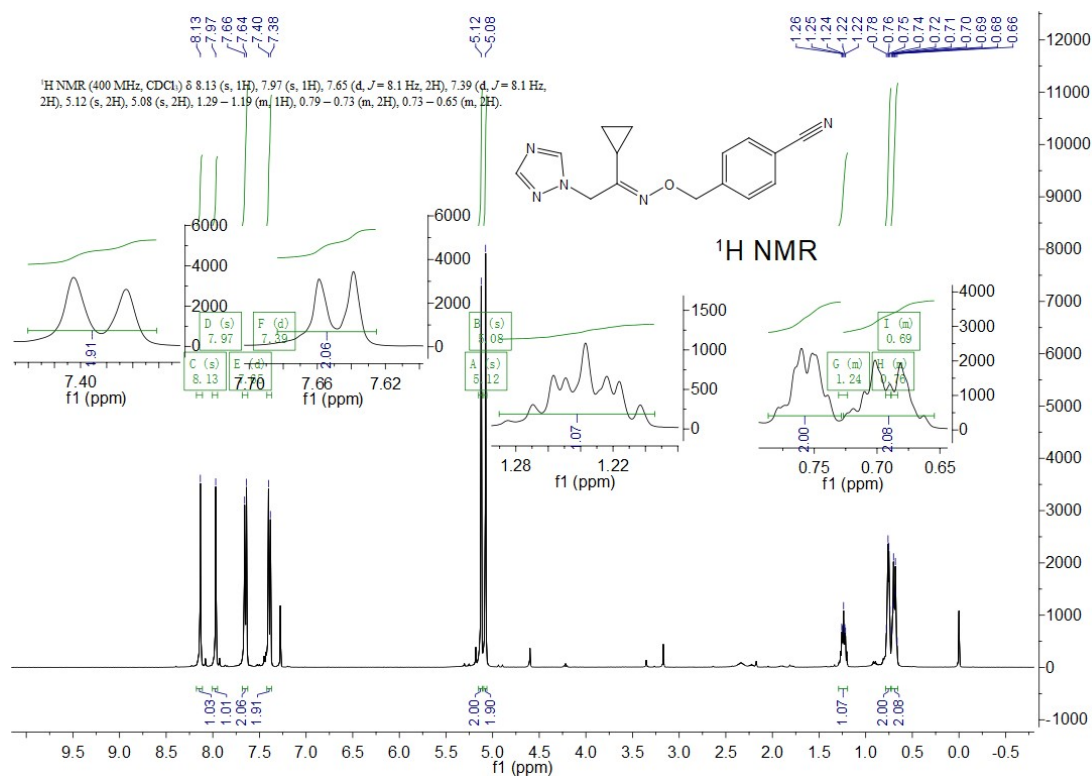


Figure 60. ¹H NMR spectrum of title compound 5s

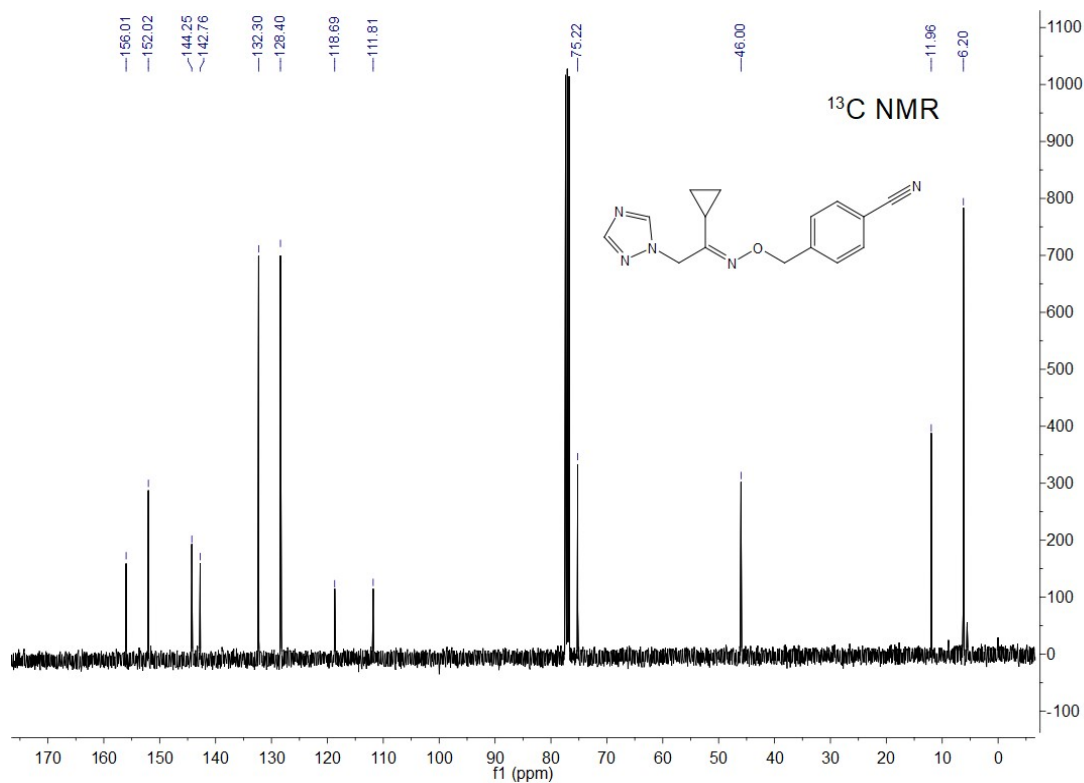


Figure 61. ¹³C NMR spectrum of title compound 5s

Spectrum from A18.wiff (sample 1) - Sample18, Experiment 1, +TOF MS (80 - 800) from 0.090 to 0.106 min

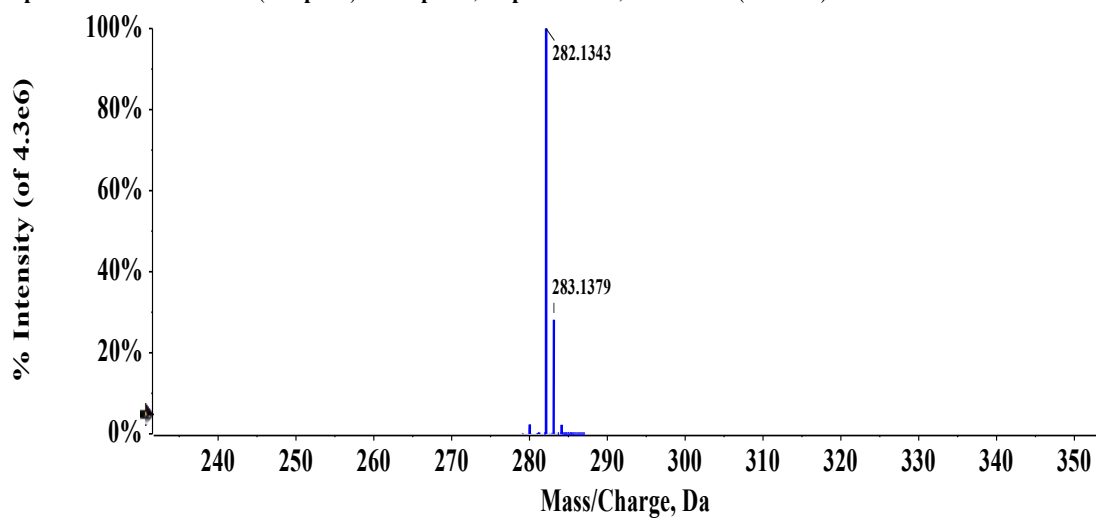


Figure 62. HRMS spectrum of title compound 5s

Compound 5t

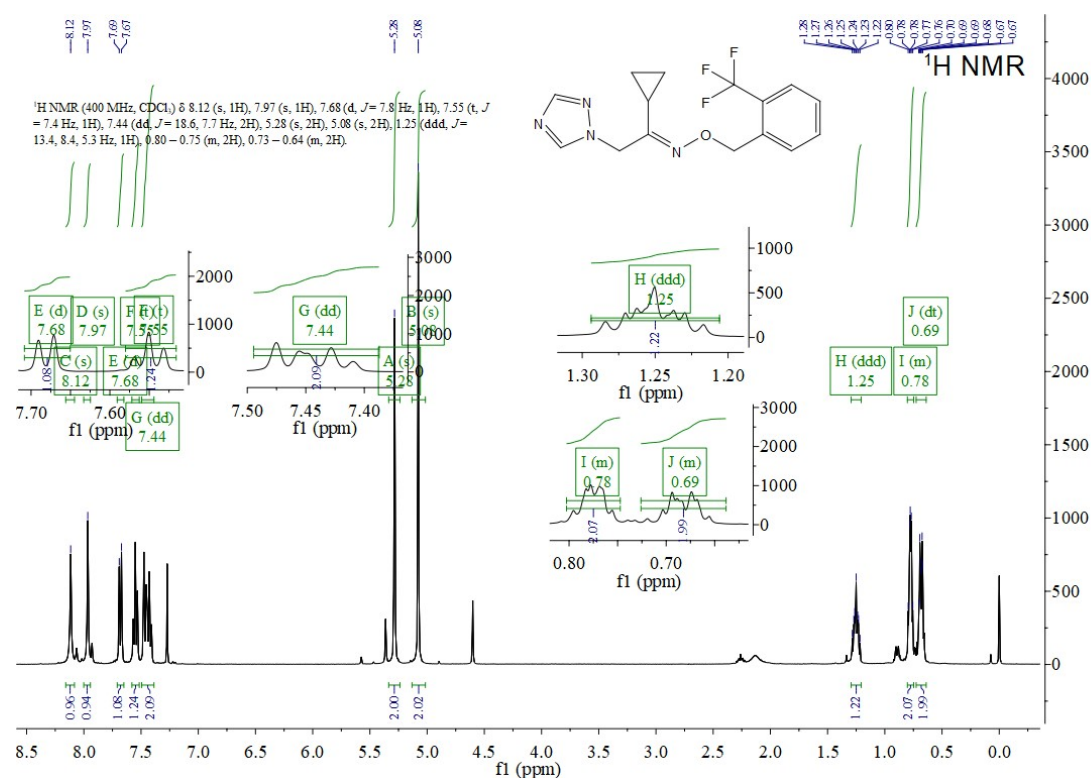


Figure 63. ¹H NMR spectrum of title compound 5t

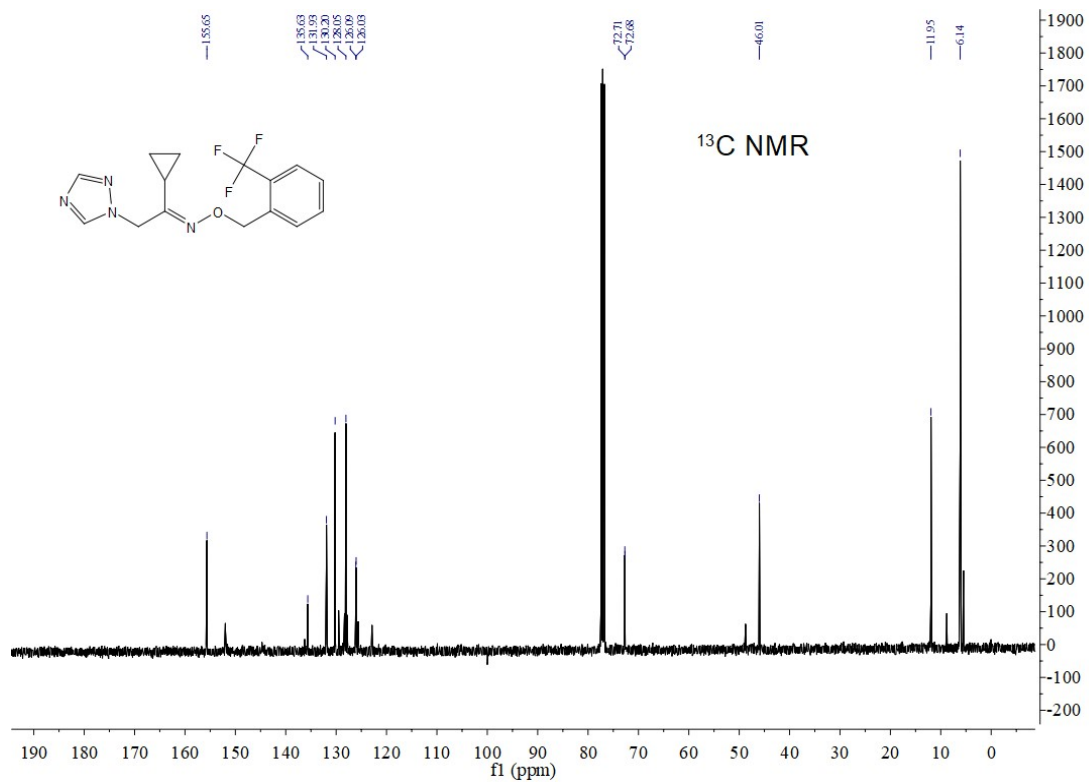


Figure 64. ¹³C NMR spectrum of title compound 5t

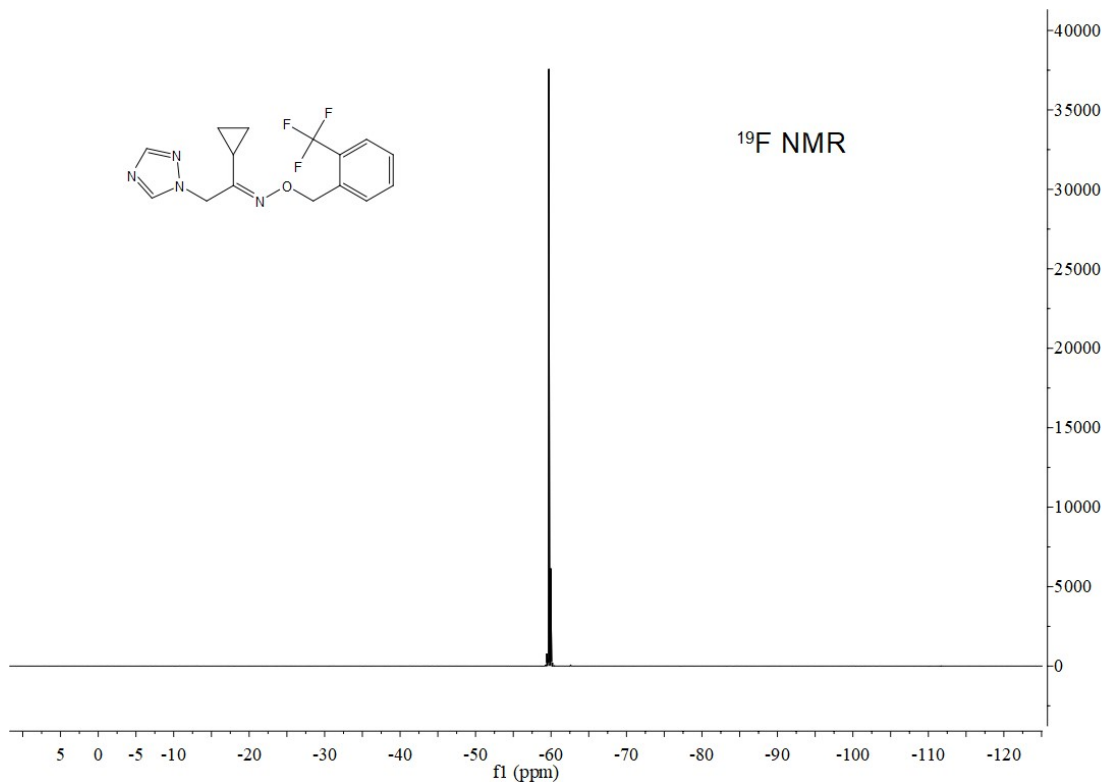


Figure 65. ¹⁹F NMR spectrum of title compound 5t

Spectrum from A19.wiff (sample 1) - Sample19, Experiment 1, +TOF MS (80 - 800) from 0.091 to 0.108 min

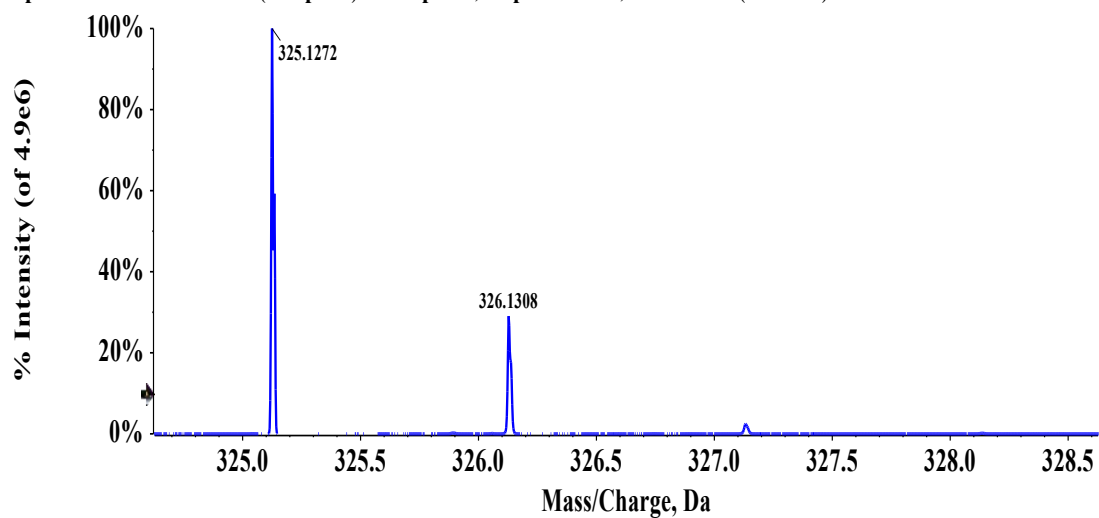


Figure 66. HRMS spectrum of title compound 5t

Compound 5u

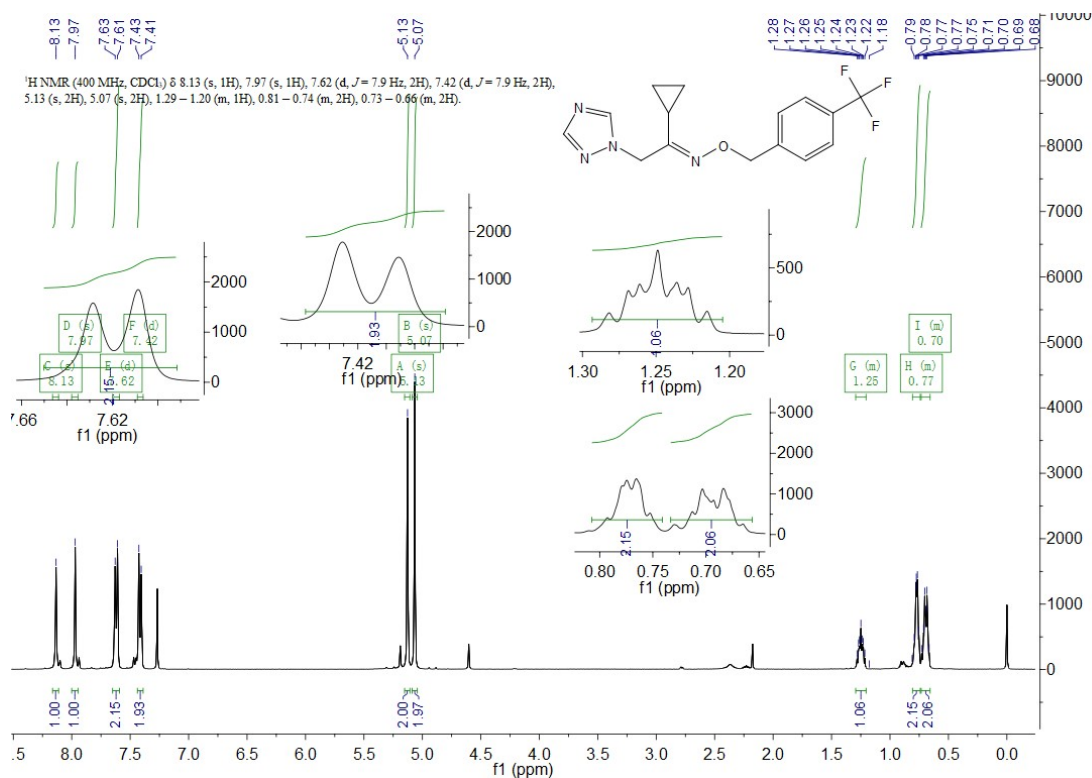


Figure 67. ¹H NMR spectrum of title compound 5u

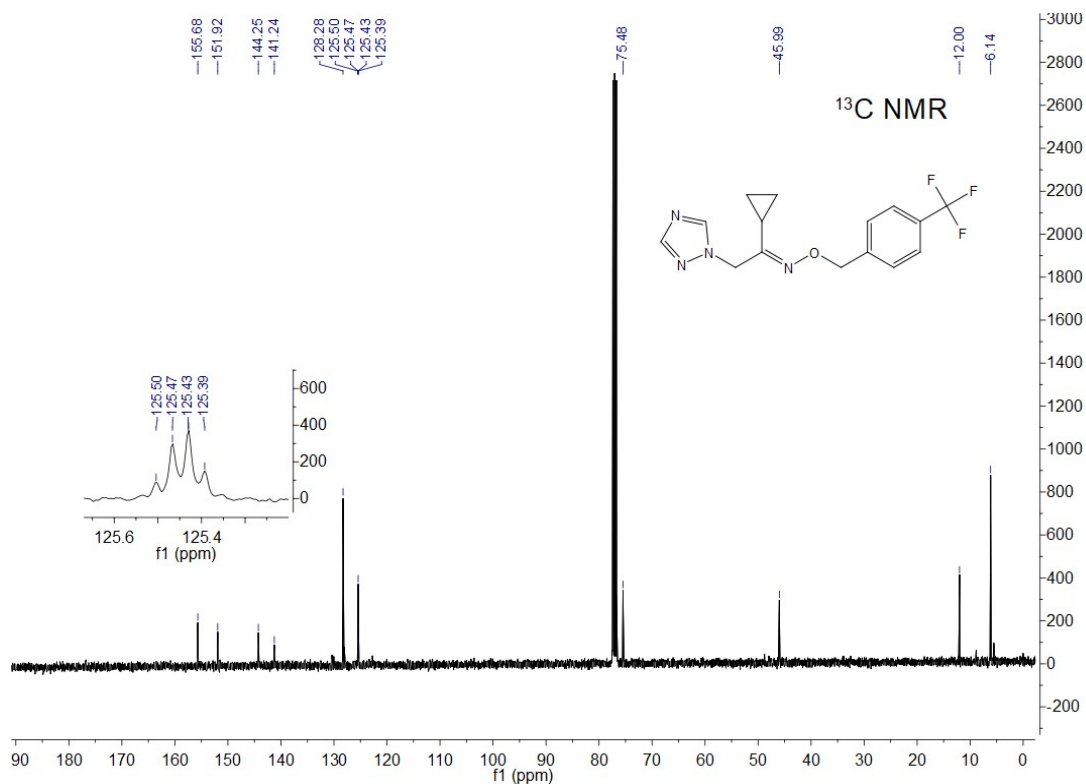


Figure 68. ¹³C NMR spectrum of title compound 5u

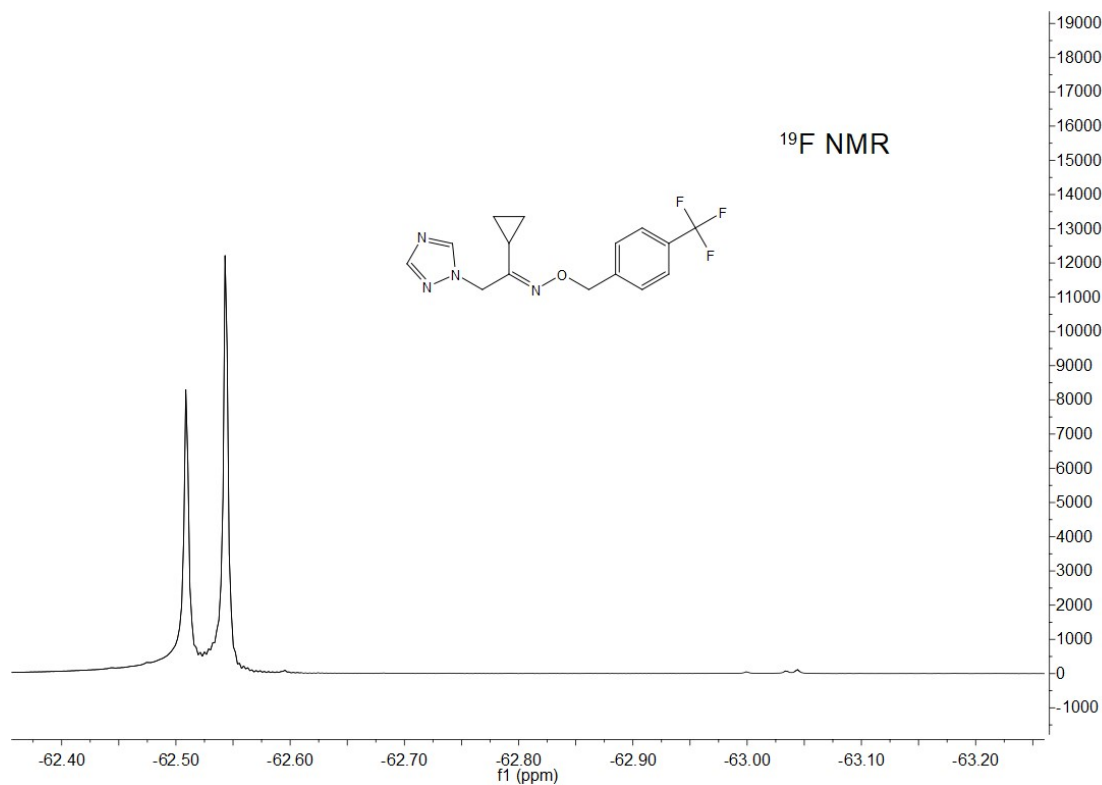


Figure 69. ¹⁹F NMR spectrum of title compound 5u

Spectrum from A21.wiff (sample 1) - Sample21, Experiment 1, +TOF MS (80 - 800) from 0.090 to 0.107 min

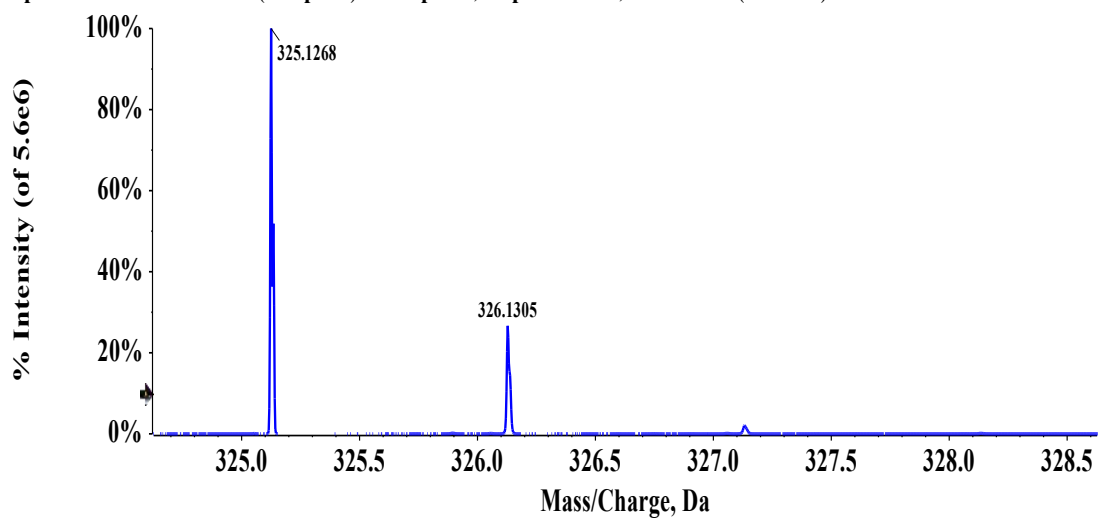


Figure 70. HRMS spectrum of title compound 5u

Compound 5v

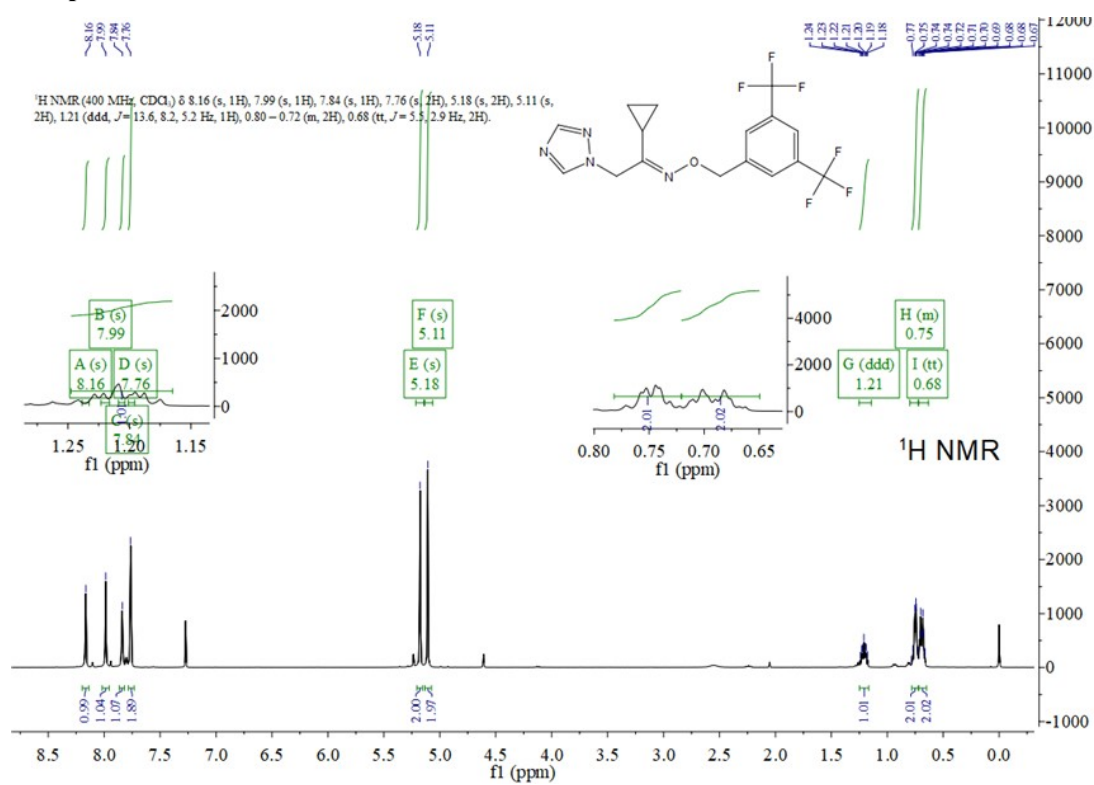


Figure 71. ¹H NMR spectrum of title compound 5v

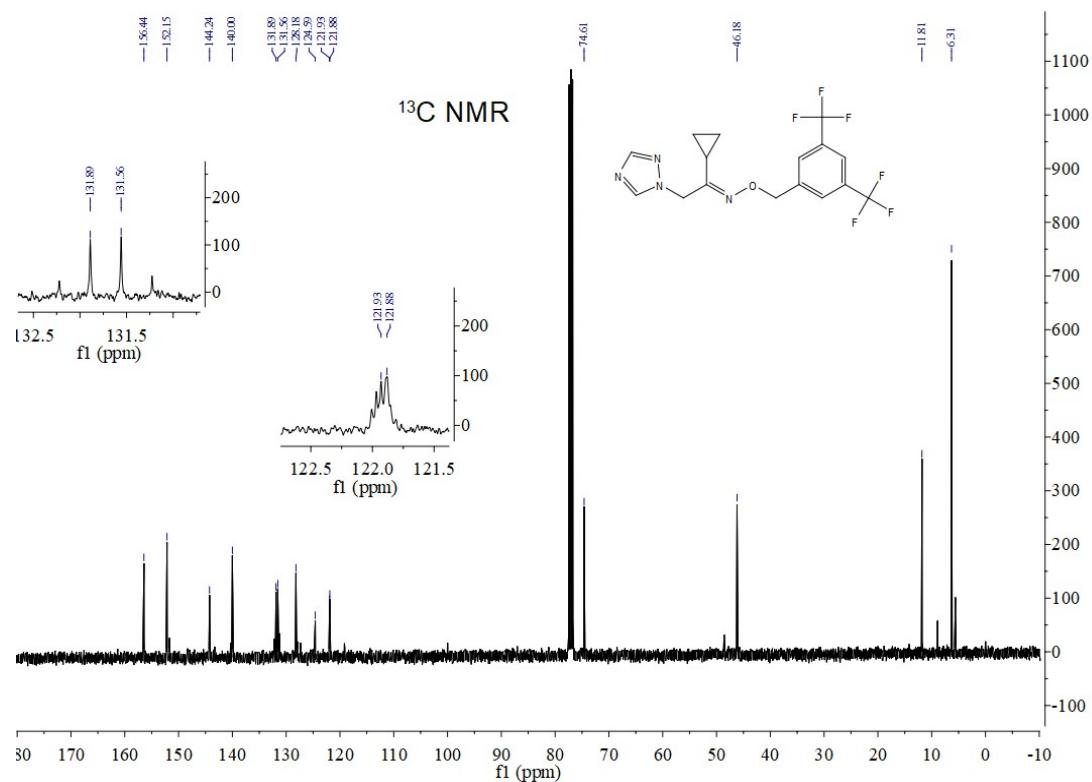


Figure 72. ¹³C NMR spectrum of title compound 5v

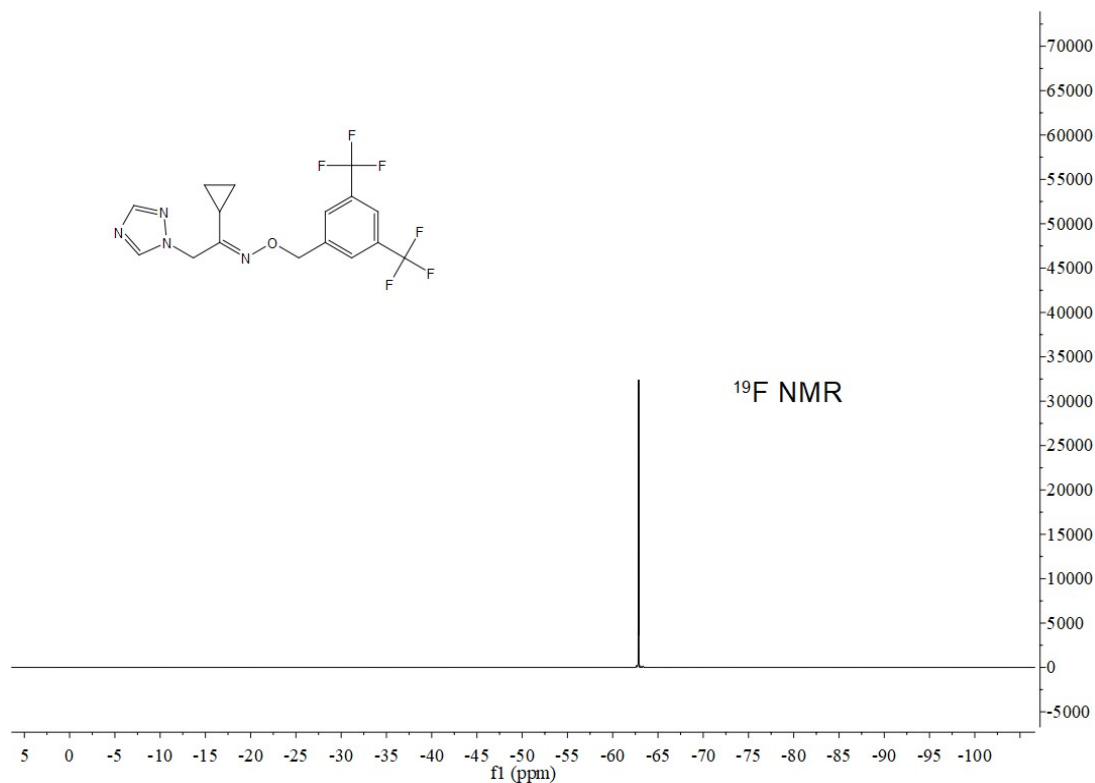


Figure 73. ¹⁹F NMR spectrum of title compound 5v

Spectrum from A20.wiff (sample 1) - Sample20, Experiment 1, +TOF MS (80 - 800) from 0.090 to 0.107 min

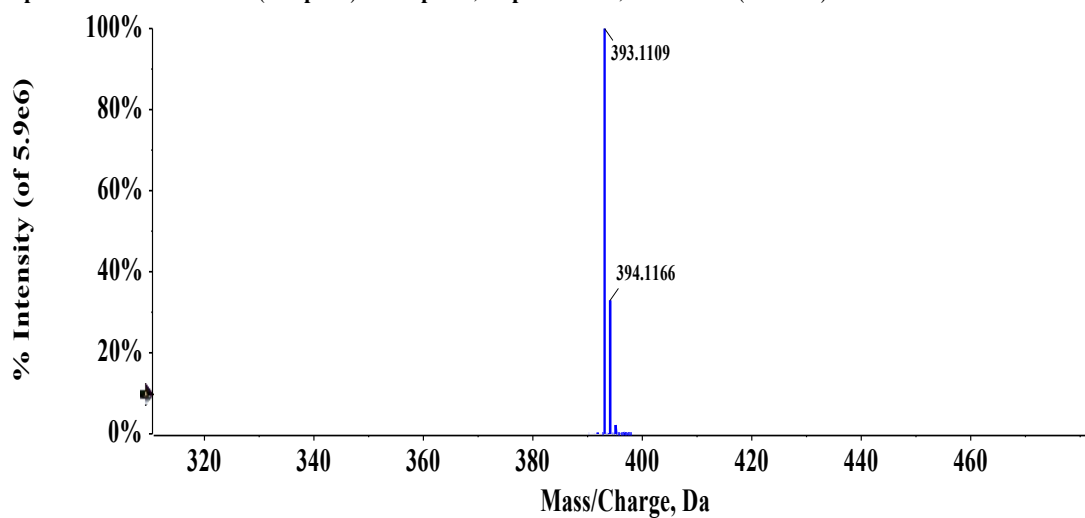


Figure 74. HRMS spectrum of title compound 5v

Compound 5w

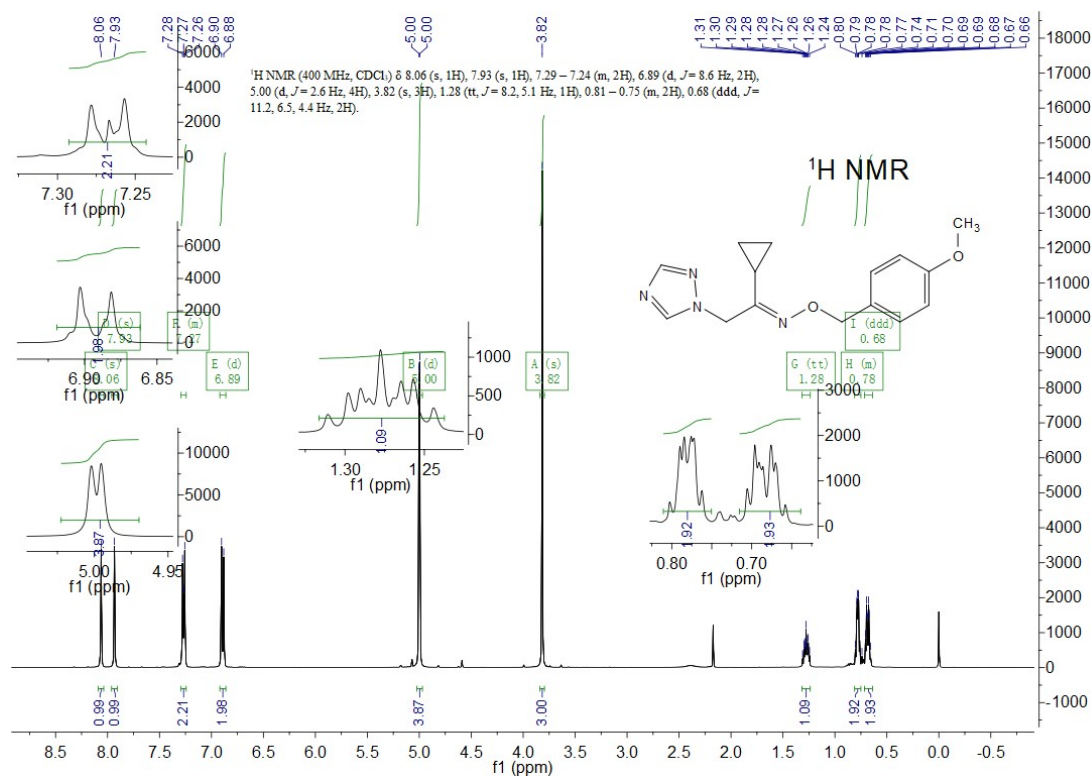


Figure 75. ¹H NMR spectrum of title compound 5w

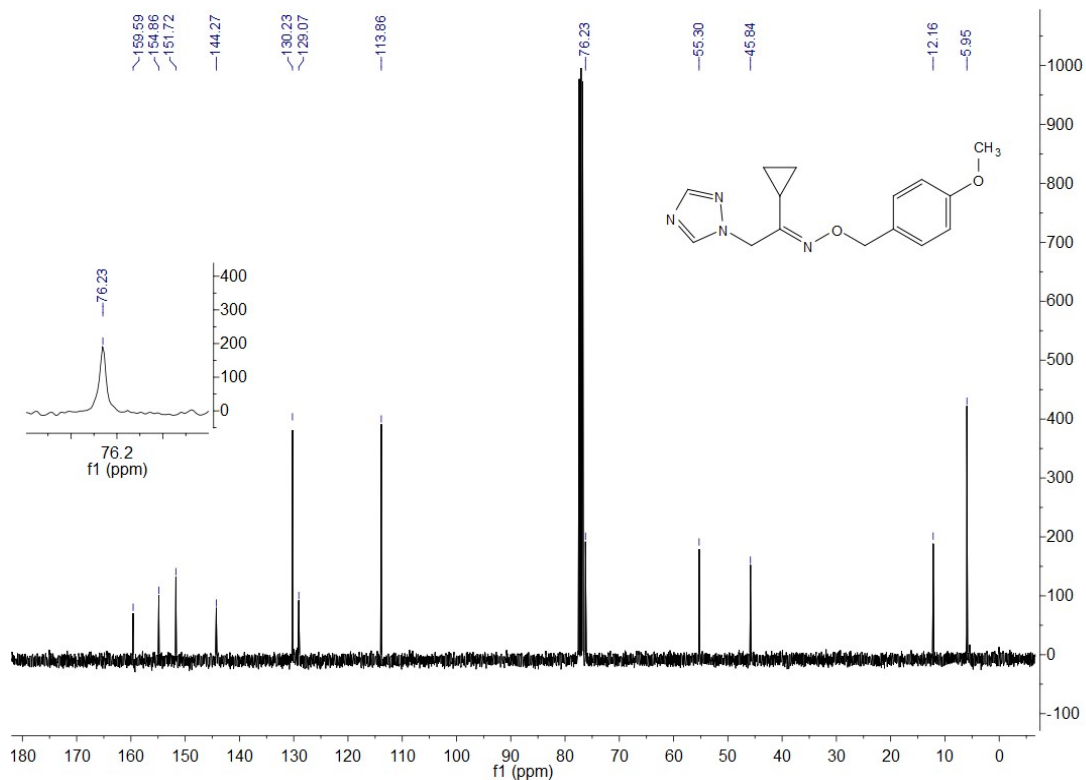


Figure 76. ^{13}C NMR spectrum of title compound 5w

Spectrum from A22.wiff (sample 1) - Sample22, Experiment 1, +TOF MS (80 - 800) from 0.090 to 0.107 min

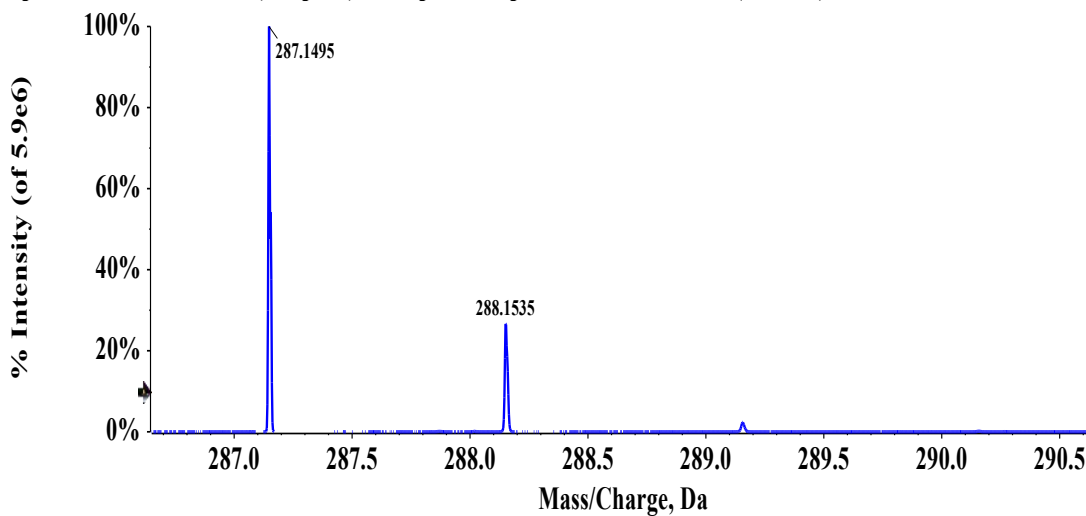


Figure 77. HRMS spectrum of title compound 5w

Compound 5x

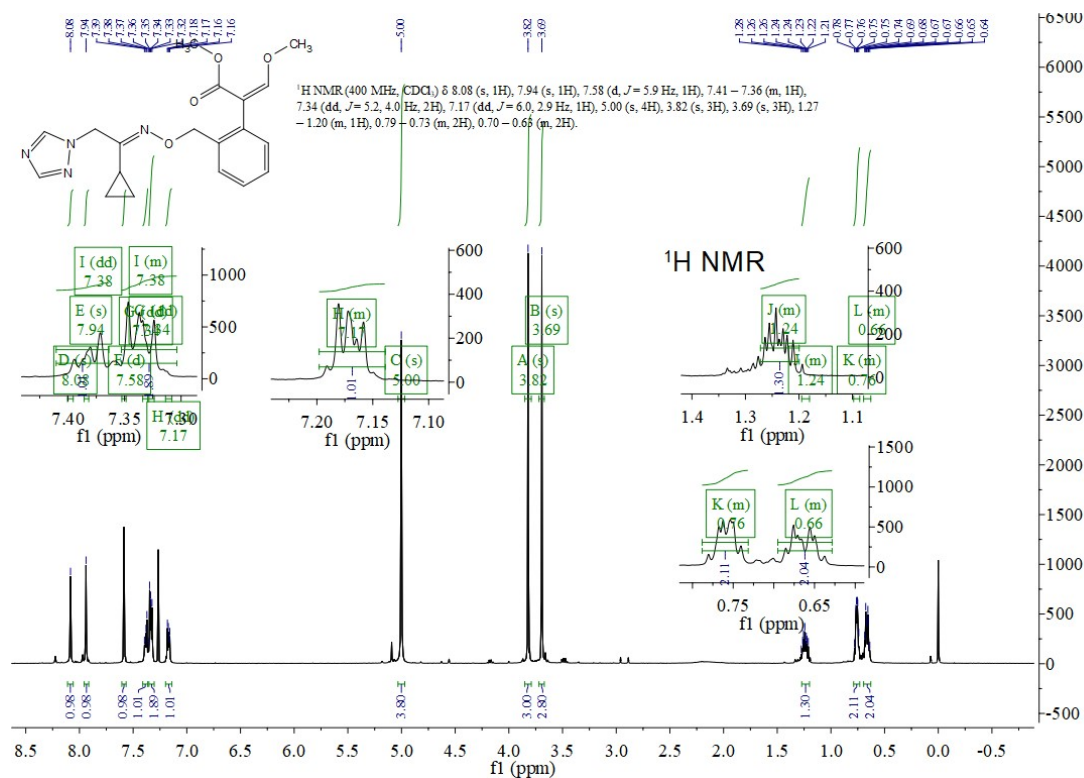


Figure 78. ¹H NMR spectrum of intermediate 5x

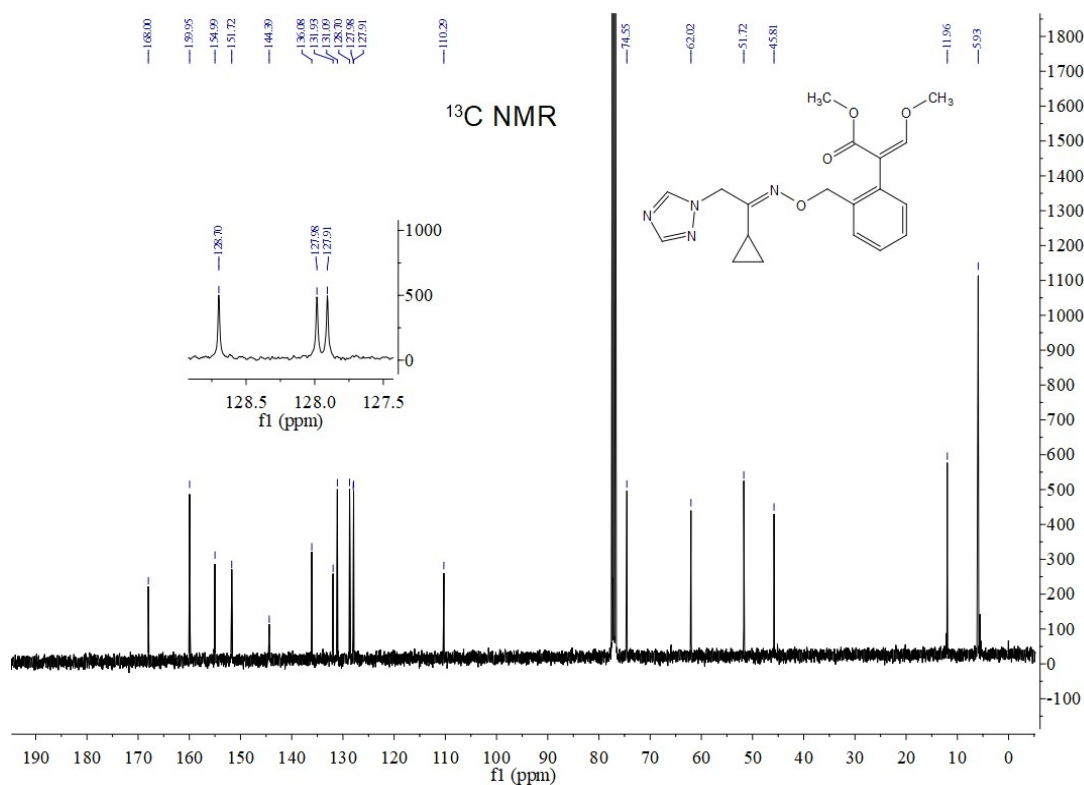


Figure 79. ¹³C NMR spectrum of title compound 5x

Spectrum from A23.wiff (sample 1) - Sample23, Experiment 1, +TOF MS (80 - 800) from 0.090 to 0.107 min

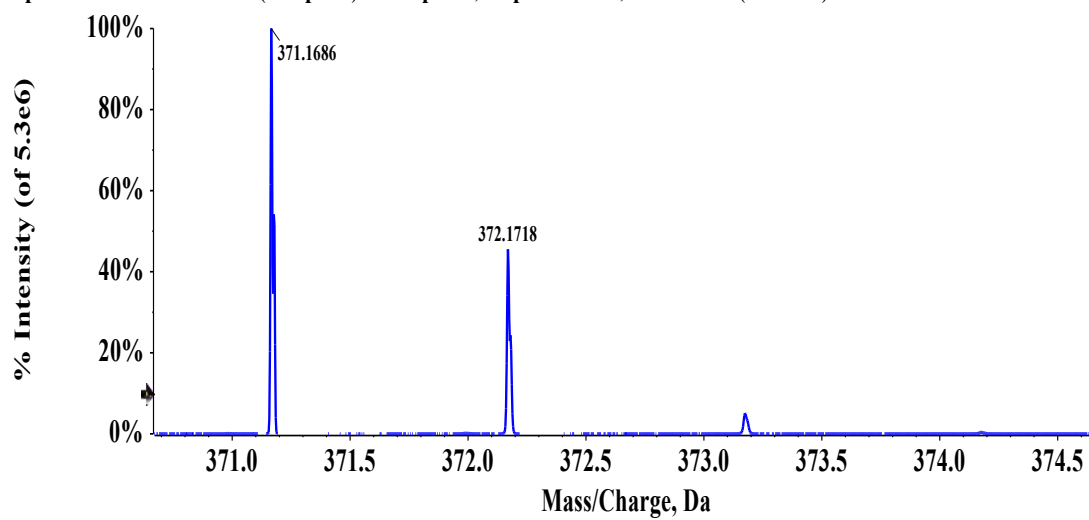


Figure 80. HRMS spectrum of title compound 5x

2 Molecular docking related information

2.1 Protein sequence of *FgCYP51*

```
>tr|I6YDU0|I6YDU0_GIBZA Cyp51A OS=Gibberella zeae OX=5518 PE=3
SV=1MFHLLIYPLWVLVALFAVIIANLLYQQLPRRPDEPPLVFHWFPFFGNNAVAYGLDPCG
FFEKCREKHGVDVFTFILFGRKIVACLGVGDNDFVLNSRLQDANAEEVYGPLTIPVFGSDV
VYDCPN SKLMEQKKFVKFGLTQKALESHVQLIEREVLDYVETDPSFSGRTSTIDVPKAMA
EITIFTASRSLQGEEVRRKLTAEFAALYHDLDLGFRPVNFLFPWLPLPHNRKRDAAHIKMR
EVYMDIINDRRKGGIRTEDGTDMIANLMGCTYKNGQPVPDKEIAHMMITLLMAGQHSSS
SASSWIVLHLASSPDMTEELYQEQLVNLSVNGALPPLQYSDLDKLPLLQNVVKETLRVHS
SIHSILRKVKRPMQV PNSPYTITTDKVMASPTVTAMSEEFENAKTWNPHRWDNRAKEE
VDTEDVIDYGYGAVSKGKSPYLPFGAGRHRGCEKFAFVNLGVIVATLVRNFRRLSTIDG
RPGVPETDYTSLFSRPAQPAFIRWERRKKI
```

2.2 Ramachandran plots of constructed protein *FgCYP51*

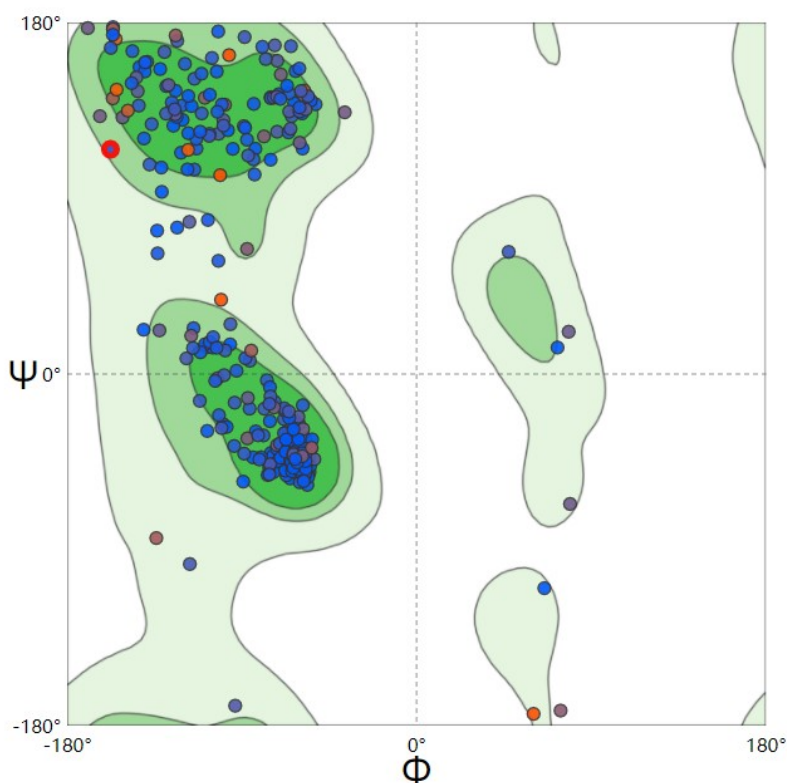


Figure 81. Ramachandran plots of constructed protein *FgCYP51*

2.3 Composite image of 4YUM and constructed protein *FgCYP51*

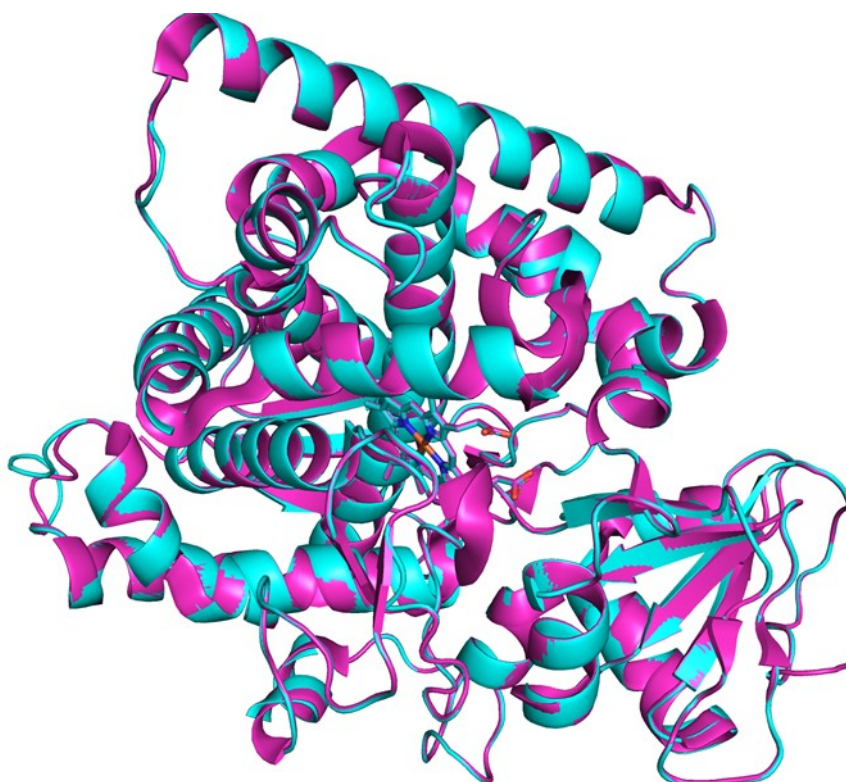


Figure 82. Composite image of 4yum (blue) and constructed protein (purple) *FgCYP51*

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

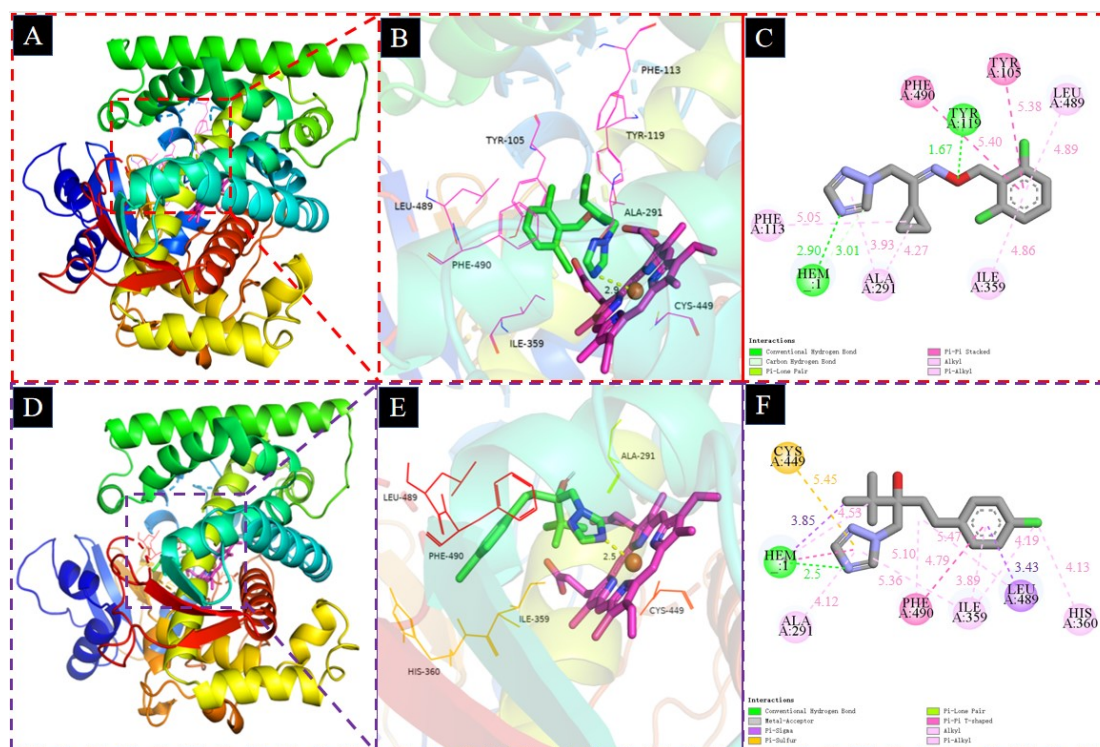


Figure 83. Molecular docking diagram of compound (*E*)-5k (A–C) and (*S*)-tebuconazole (D–F)

