

Novel fungicidal phenylethanol derivatives linking a trifluoromethyl pyrazole pharmacophore: design, synthesis, crystal structure, and biology evaluation

Lang Tai,^a Sheng-Xin Sun,^a Kai Yue,^a Jian-Qi Chai,^{ab} Shuai-Tao Hou,^{ab} Guang-Yu Dai,^a Chun-Long Yang^{*ab} and Min Chen^{*ab}

^a *Department of Chemistry, College of Sciences, Nanjing Agricultural University, Nanjing, 210095, China*

^b *Jiangsu Key Laboratory of Pesticide Science, Nanjing Agricultural University, Nanjing, 210095, China*

*Corresponding author: ycl@njau.edu.cn (C.-L. Yang); chenmin@njau.edu.cn (M. Chen)

Table of Contents

1	Spectrograms of target compounds 6a-6z	3
----------	---	----------

1 Spectrograms of target compounds 6a-6z

Compound 6a

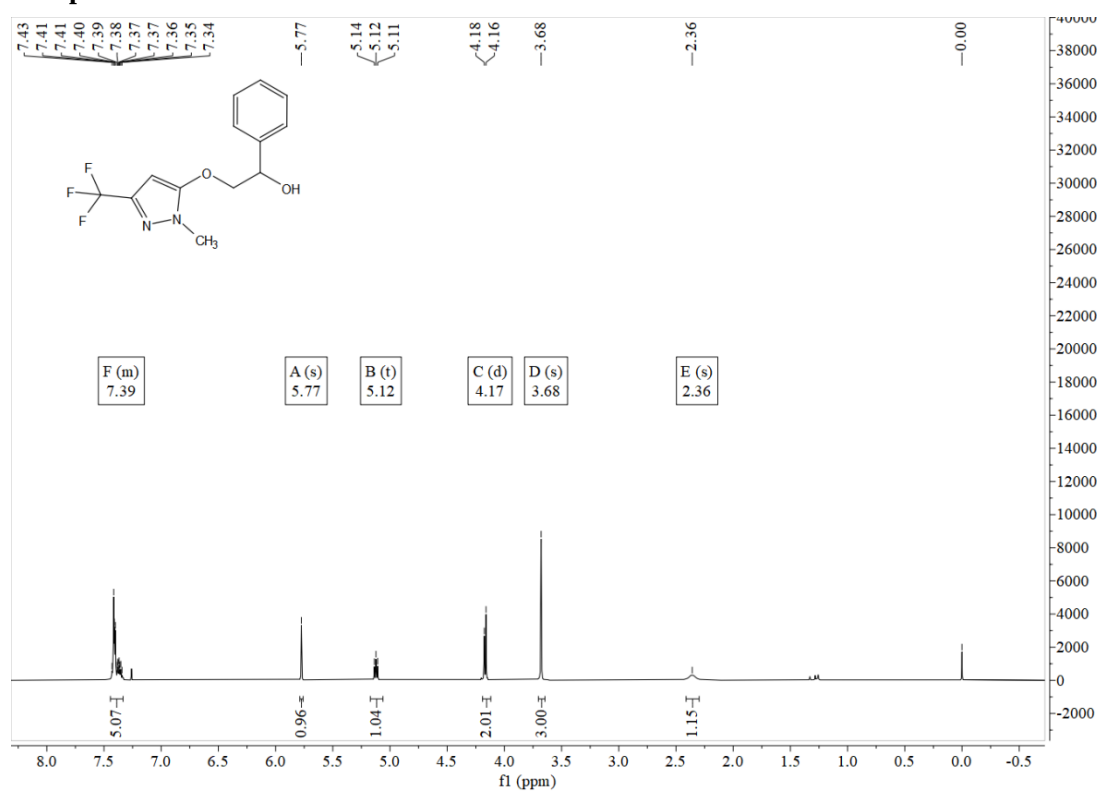


Figure 1. ¹H NMR spectrum of target compound 6a

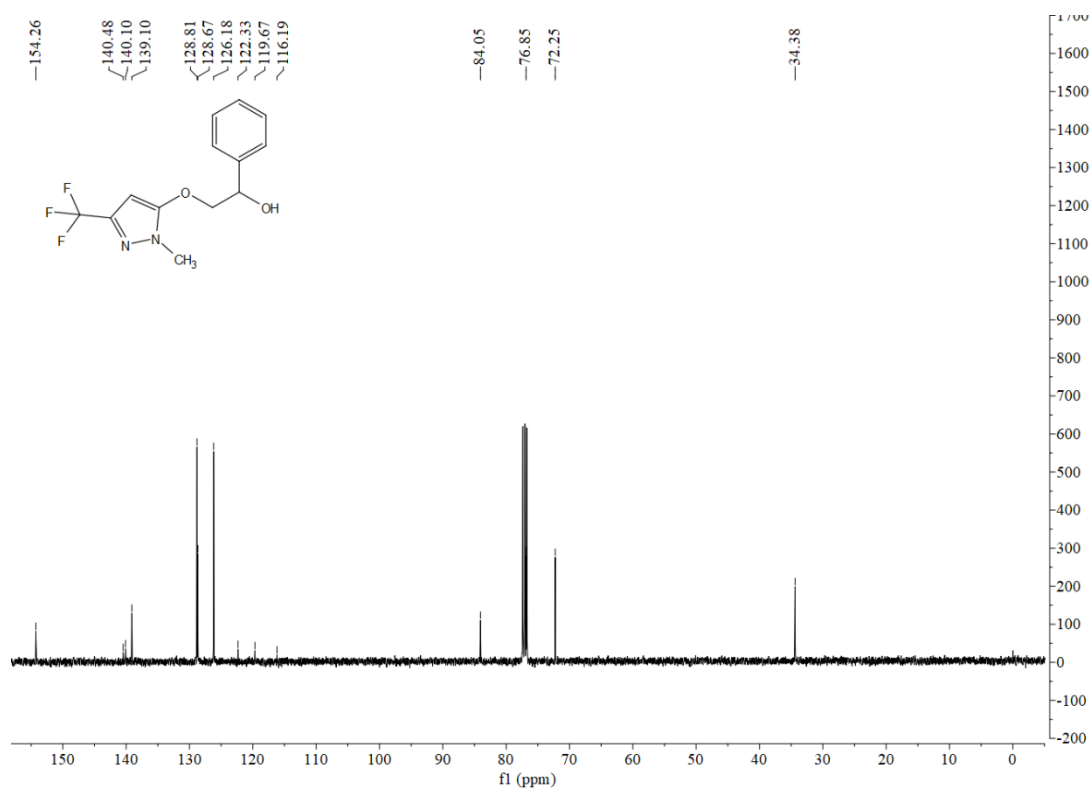


Figure 2. ¹³C NMR spectrum of target compound 6a

Spectrum from 6-4.wiff (sample 1) - Sample024, Ex...ent 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

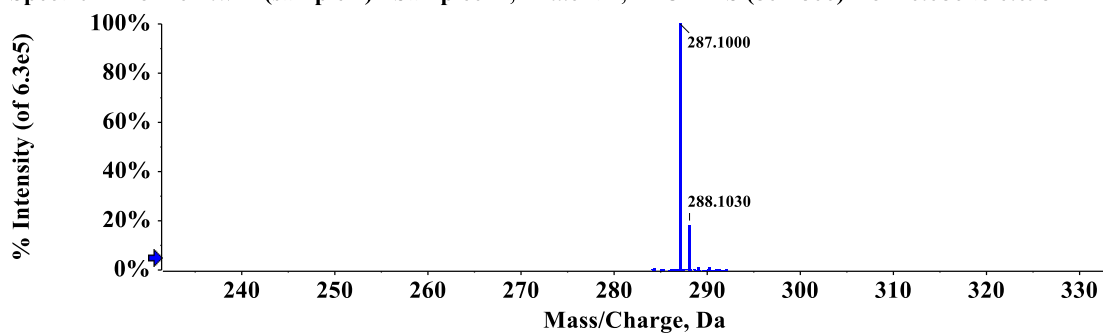


Figure 3. HRMS spectrum of target compound 6a

Compound 6b

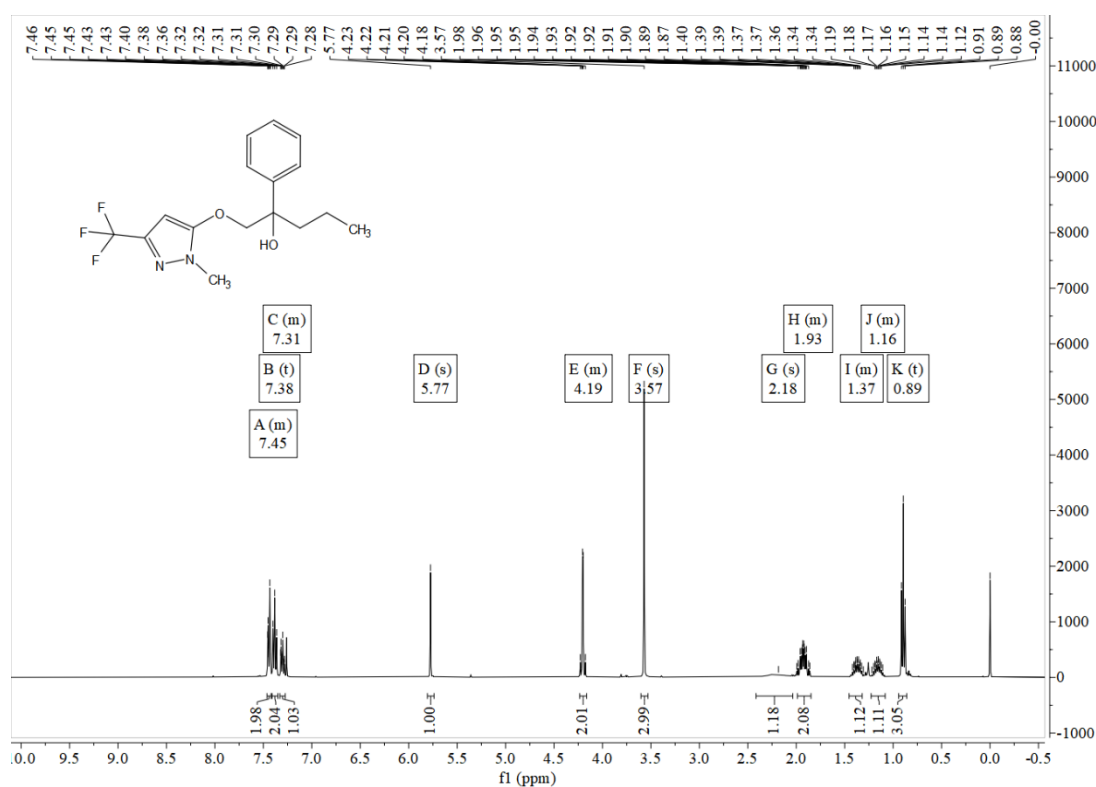


Figure 4. ¹H NMR spectrum of title target 6b

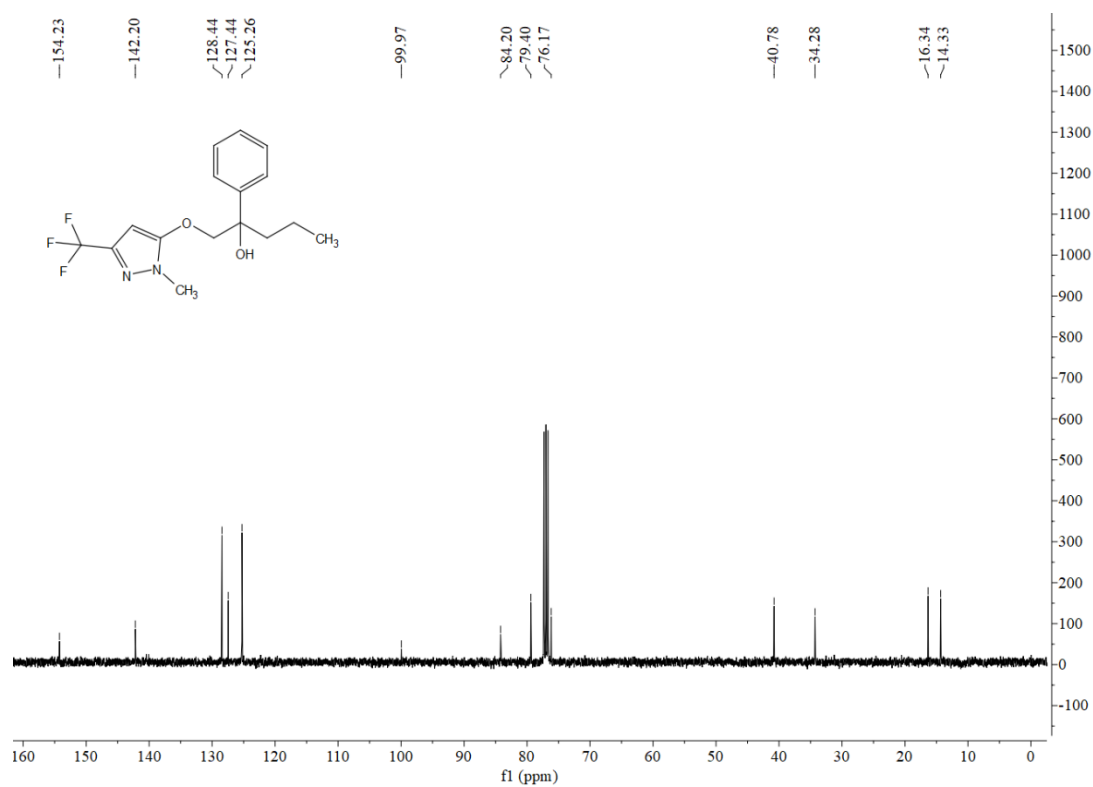


Figure 5. ¹³C NMR spectrum of target compound 6b

Spectrum from 6-5.wiff (sample 1) - Sample025, Experiment 1, +TOF MS (80 - 800) from 0.096 min

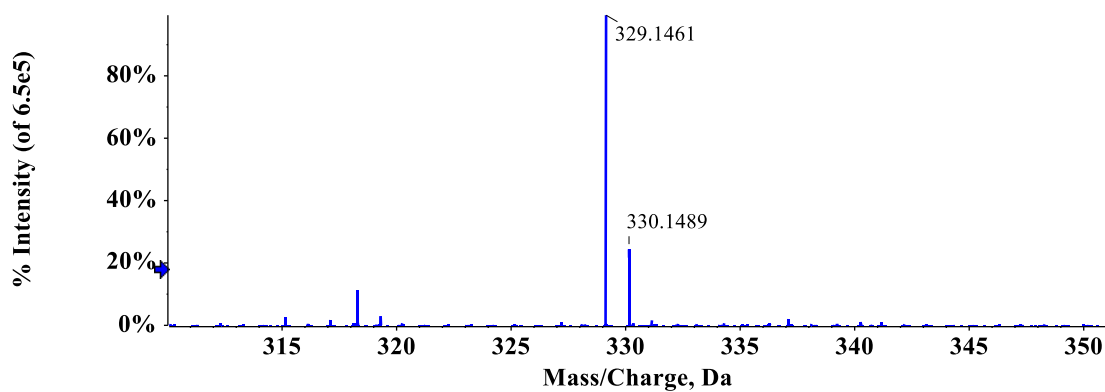


Figure 6. HRMS spectrum of target compound 6b

Compound 6c

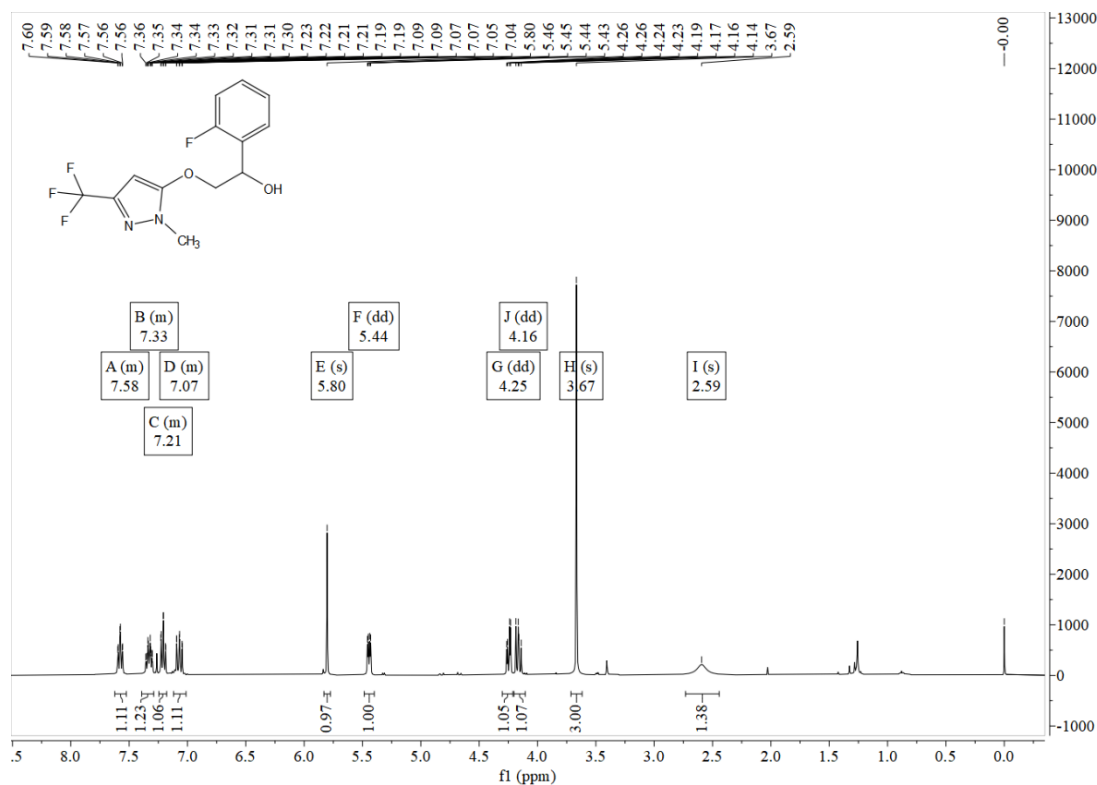


Figure 7. ¹H NMR spectrum of target compound 6c

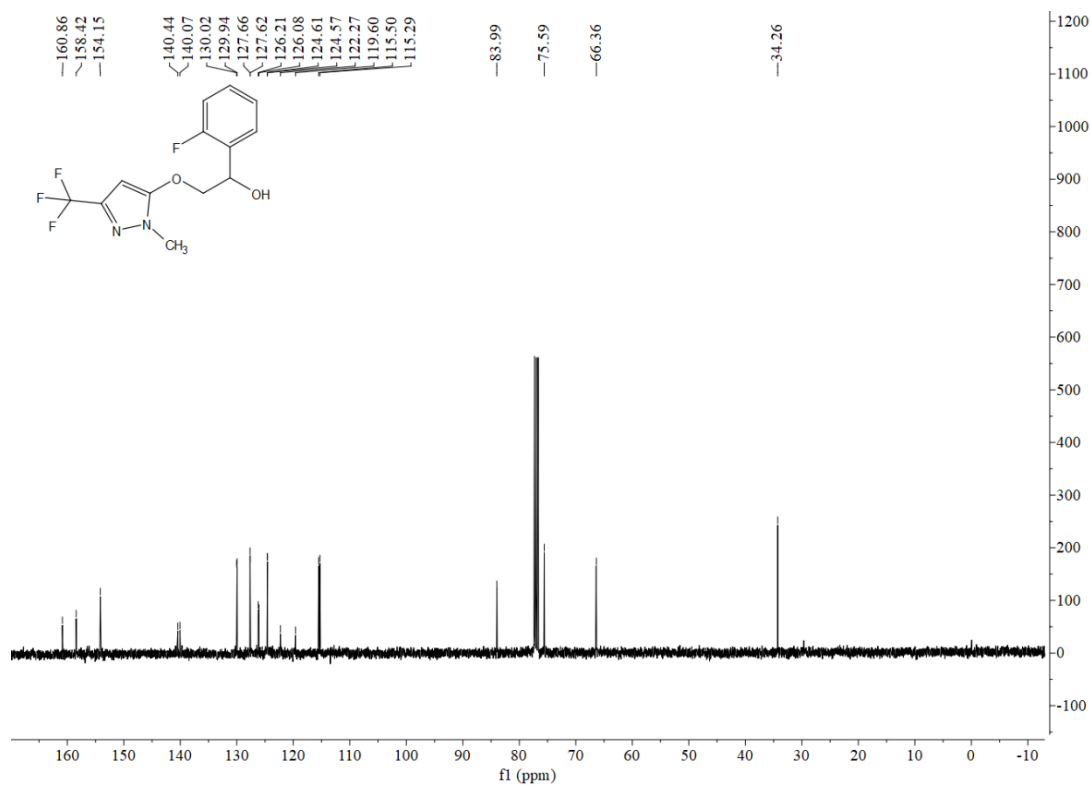


Figure 8. ¹³C NMR spectrum of target compound 6c

Spectrum from 7-2.wiff (sample 1) - Sample032, Ex...ent 1, +TOF MS (80 - 800) from 0.087 to 0.097 min

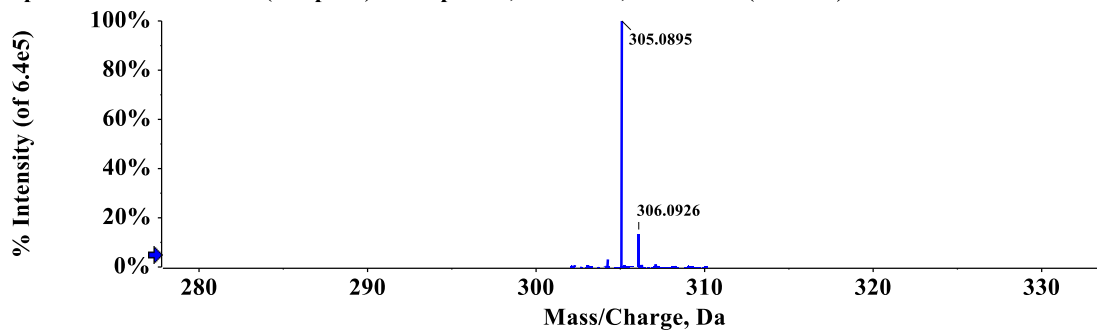


Figure 9. HRMS spectrum of target compound 6c

Compound 6d

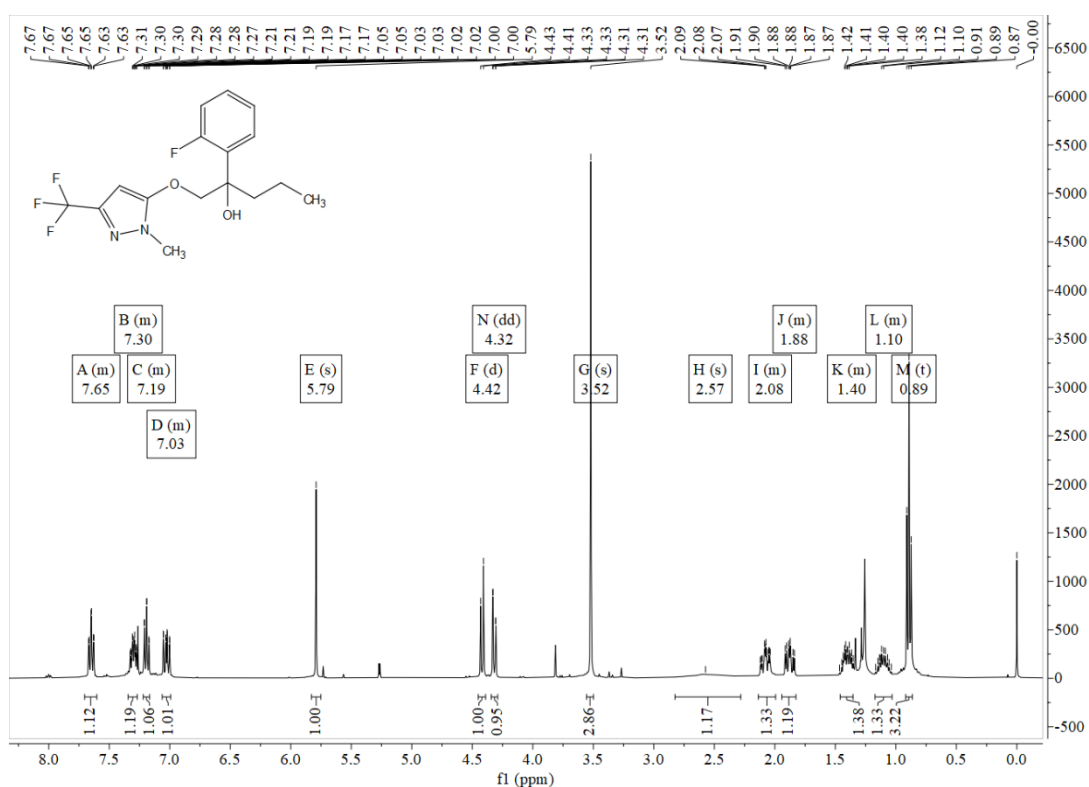


Figure 10. ¹H NMR spectrum of target compound 6d

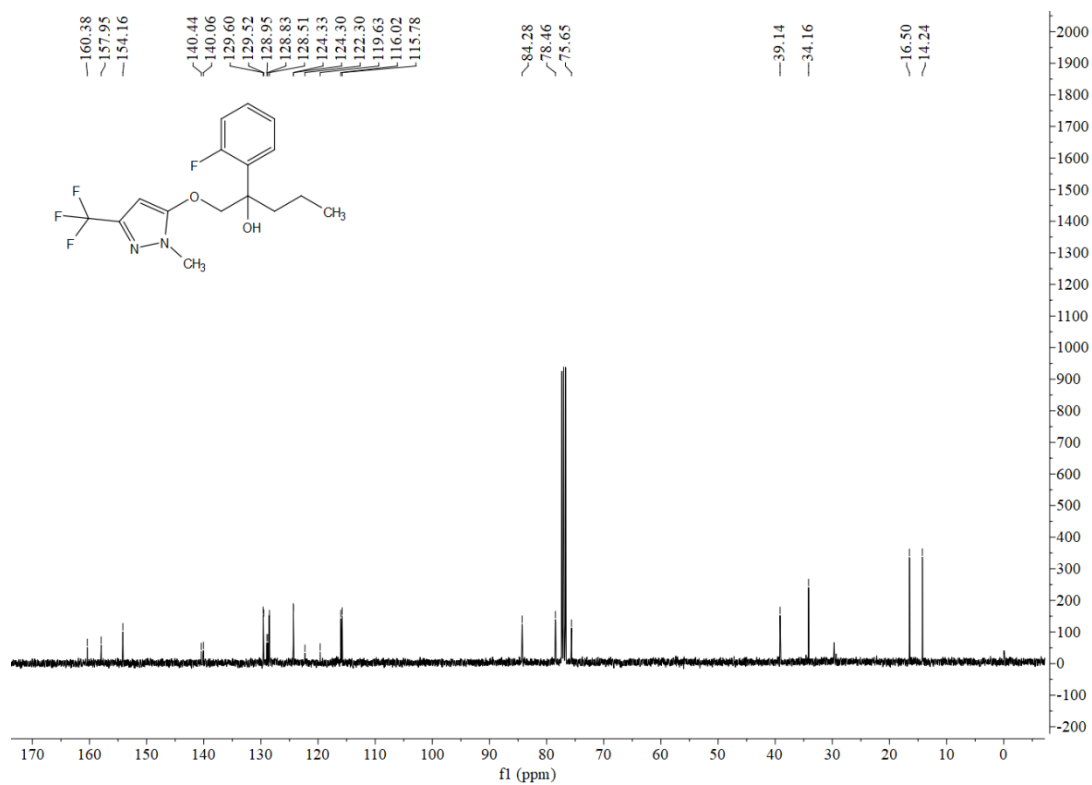


Figure 11. ¹³C NMR spectrum of target compound 6d

Spectrum from 7-1.wiff (sample 1) - Sample031, Ex...ent 1, +TOF MS (80 - 800) from 0.073 to 0.082 min

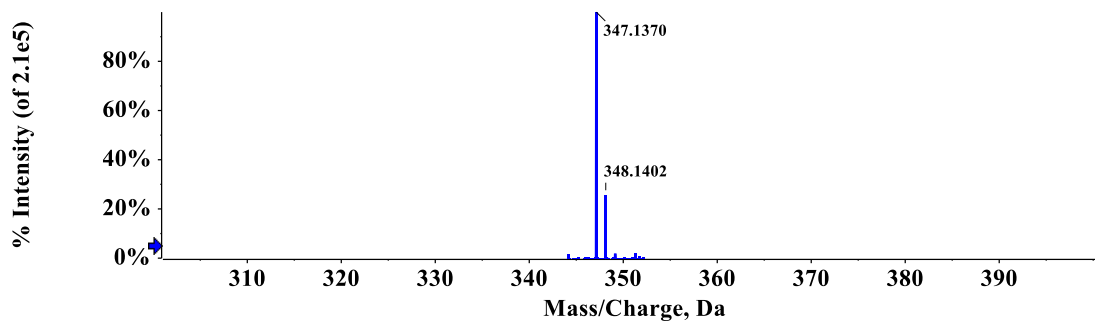


Figure 12. HRMS spectrum of target compound 6d

Compound 6e



Figure 13. ¹H NMR spectrum of target compound 6e

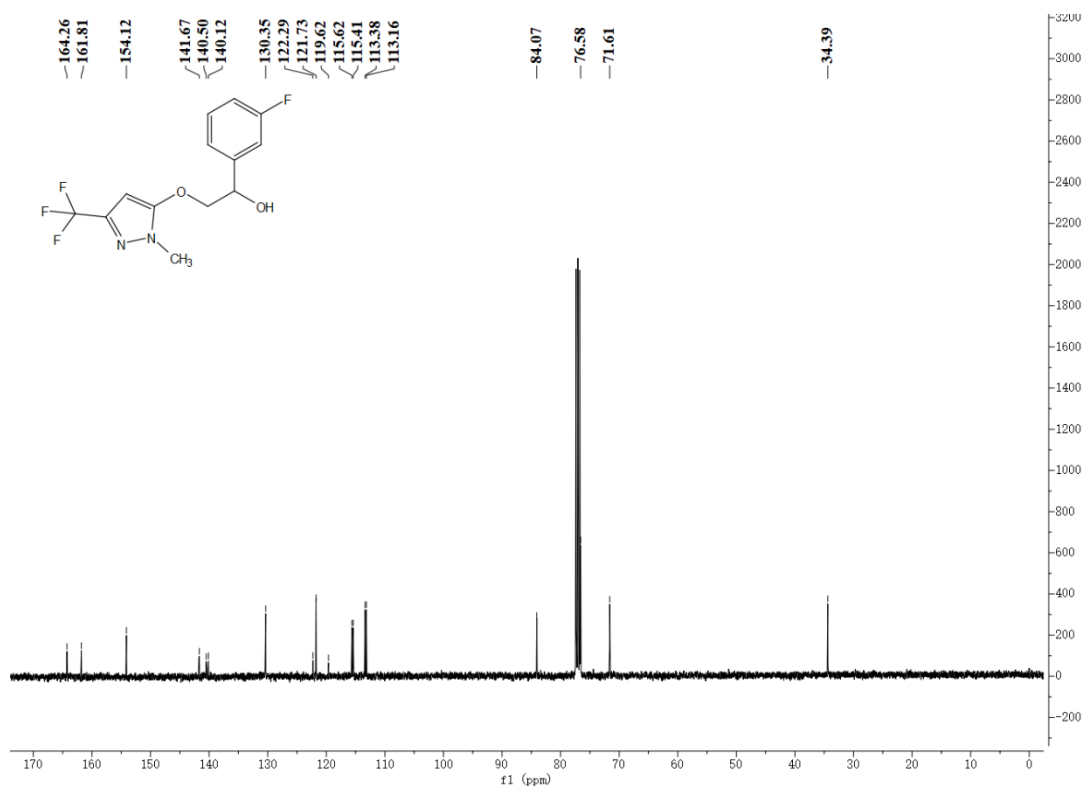


Figure 14. ¹³C NMR spectrum of target compound 6e

Spectrum from 7-6.wiff (sample 1) - Sample036, Ex...ent 1, +TOF MS (80 - 800) from 0.091 to 0.108 min

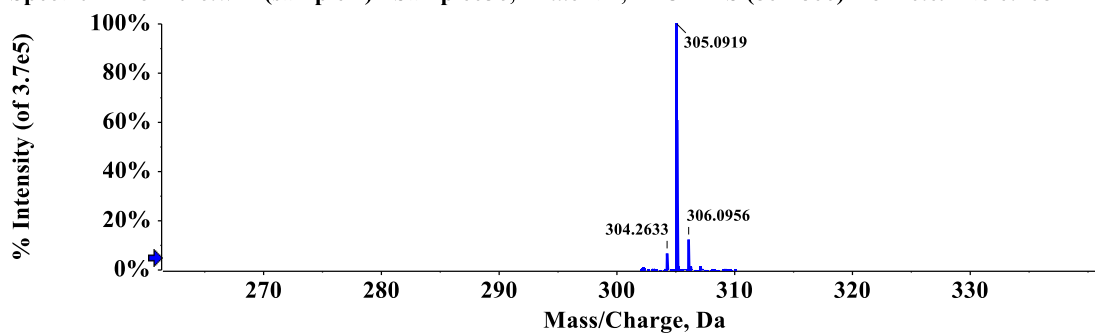


Figure 15. HRMS spectrum of target compound 6e

Compound 6f

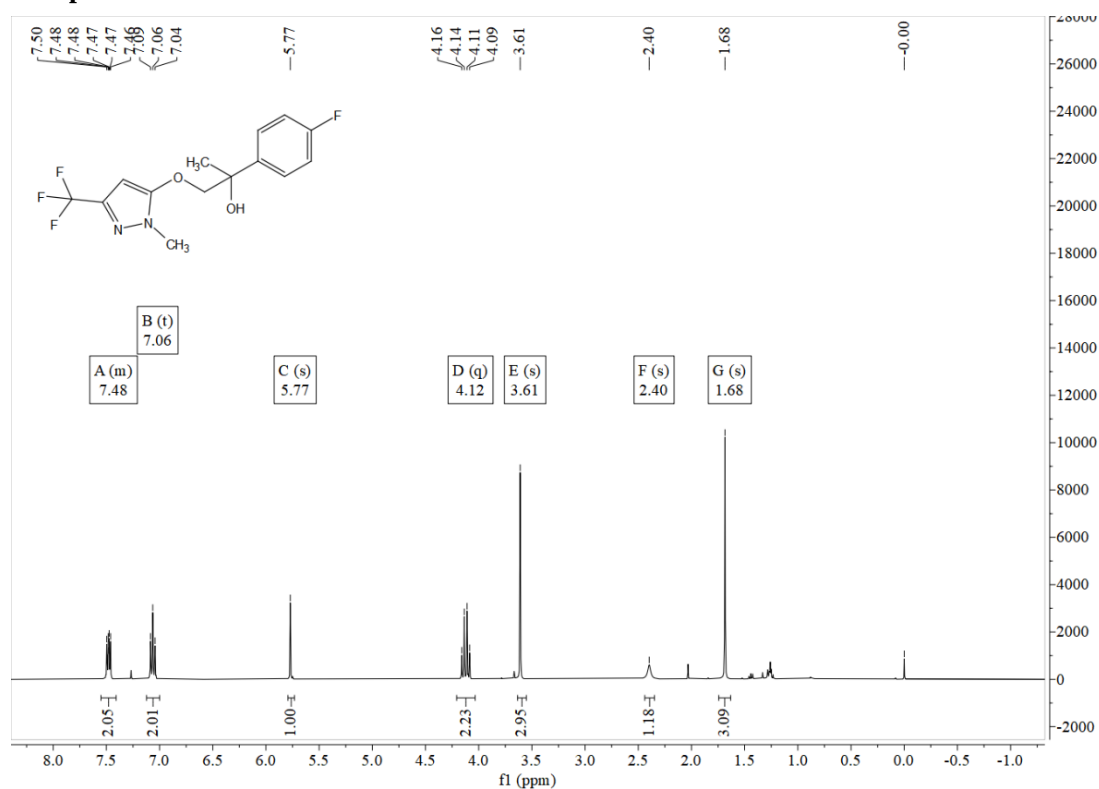


Figure 16. ¹H NMR spectrum of target compound 6f

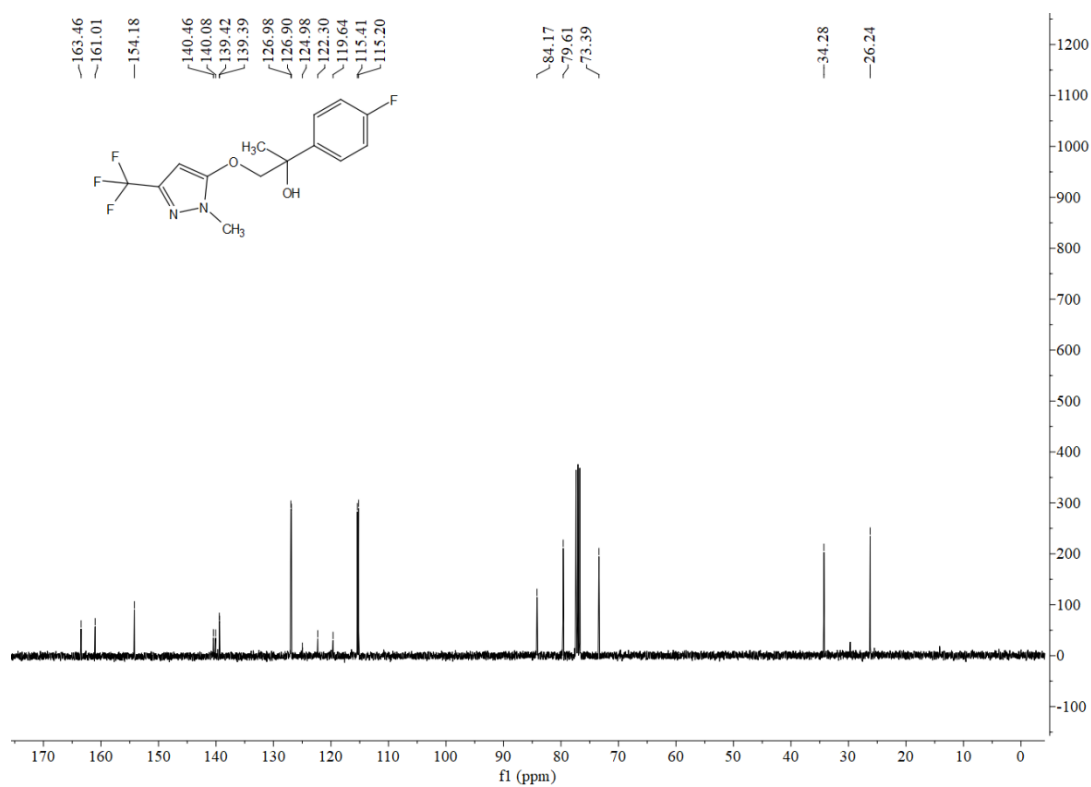


Figure 17. ¹³C NMR spectrum of target compound 6f

Spectrum from 7-3.wiff (sample 1) - Sample033, Ex...ent 1, +TOF MS (80 - 800) from 0.077 to 0.086 min

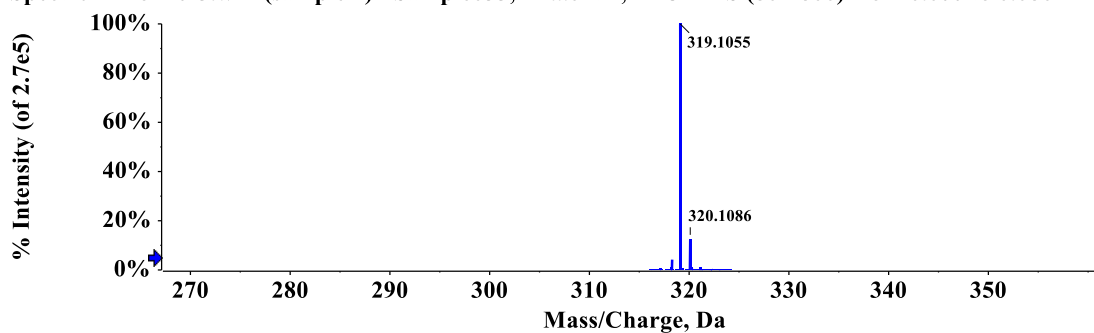


Figure 18. HRMS spectrum of target compound 6f

Compound 6g

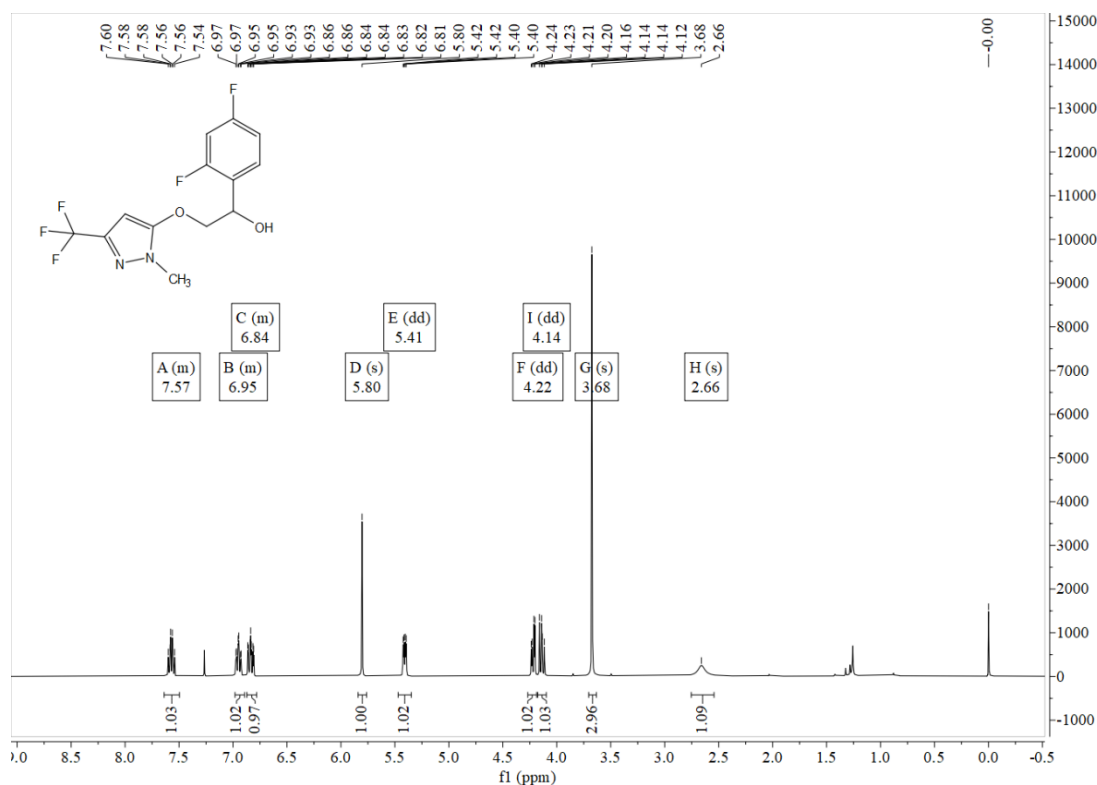


Figure 19. ¹H NMR spectrum of target compound 6g

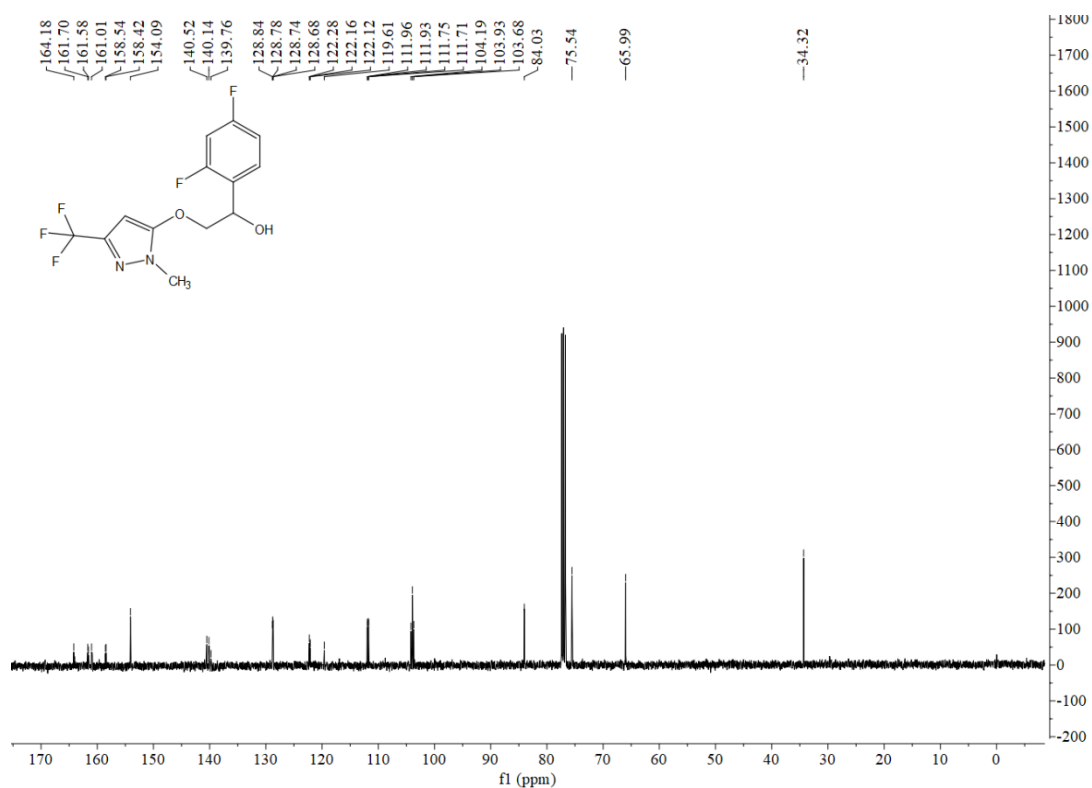


Figure 20. ¹³C NMR spectrum of target compound 6g

Mass spectrum showing relative intensity (%) versus Mass/Charge (Da). The base peak is at 323.0795 Da. Other labeled peaks include 324.0823 Da and 325.0823 Da.

Compound 6h



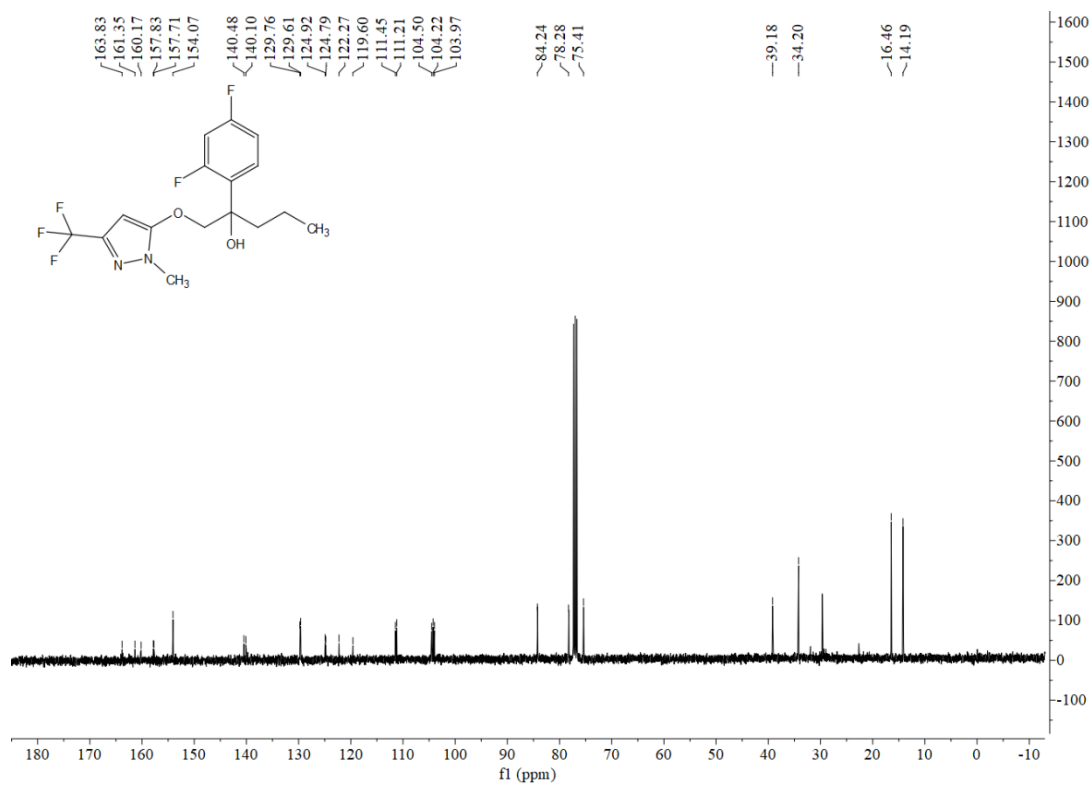


Figure 23. ¹³C NMR spectrum of target compound 6h

Spectrum from 7-4.wiff (sample 1) - Sample034, Experiment 1, +TOF MS (80 - 800) from 0.096 min

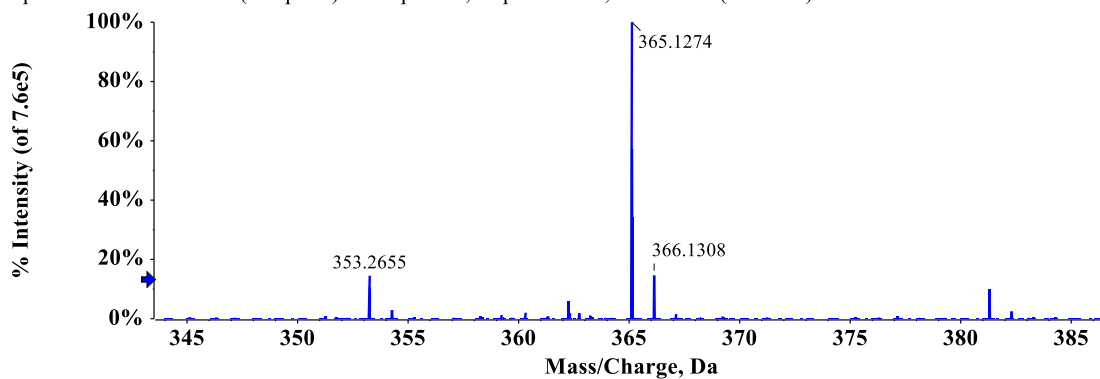


Figure 24. HRMS spectrum of target compound 6h

Compound 6i

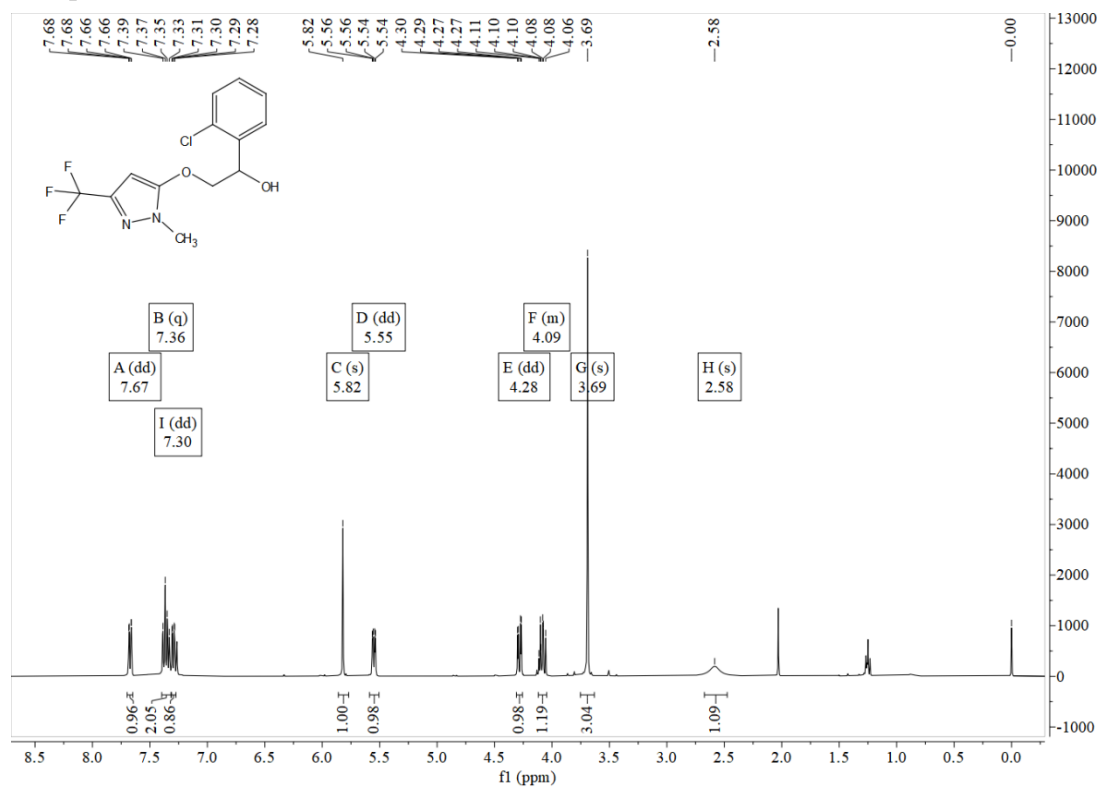


Figure 25. ¹H NMR spectrum of target compound 6i

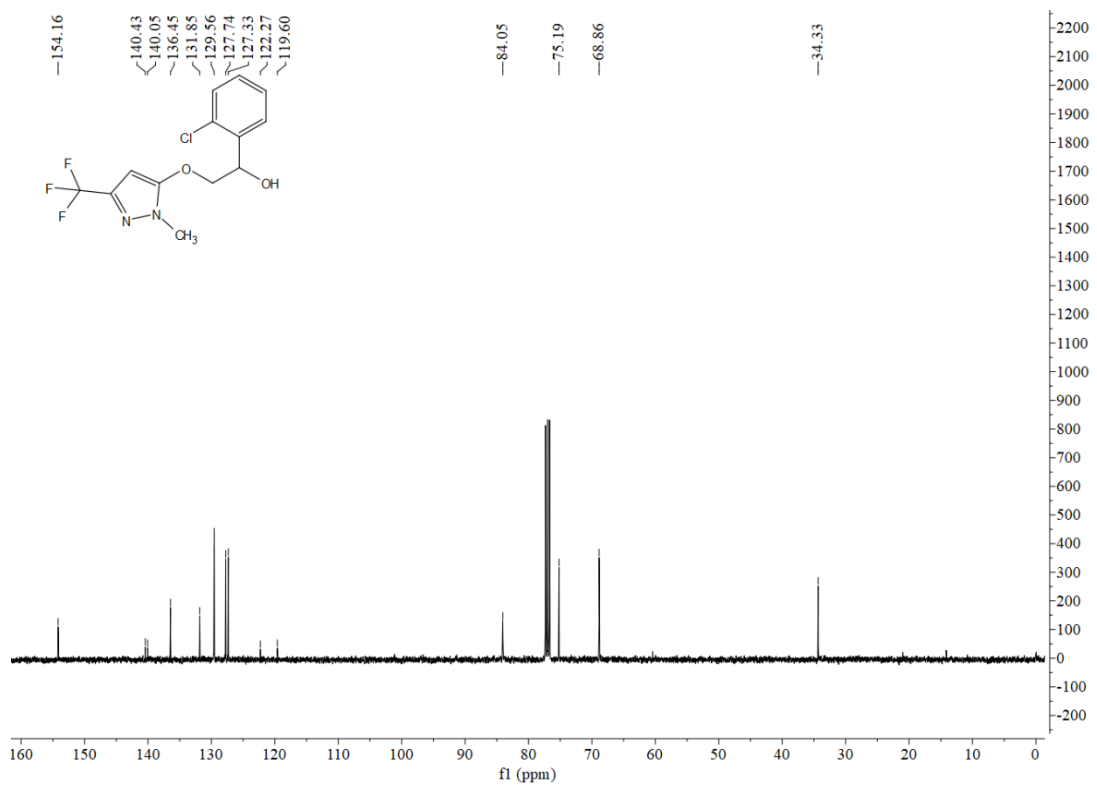


Figure 26. ¹³C NMR spectrum of target compound 6i

Spectrum from 6-1.wiff (sample 1) - Sample021, Experiment 1, +TOF MS (80 - 800) from 0.096 min

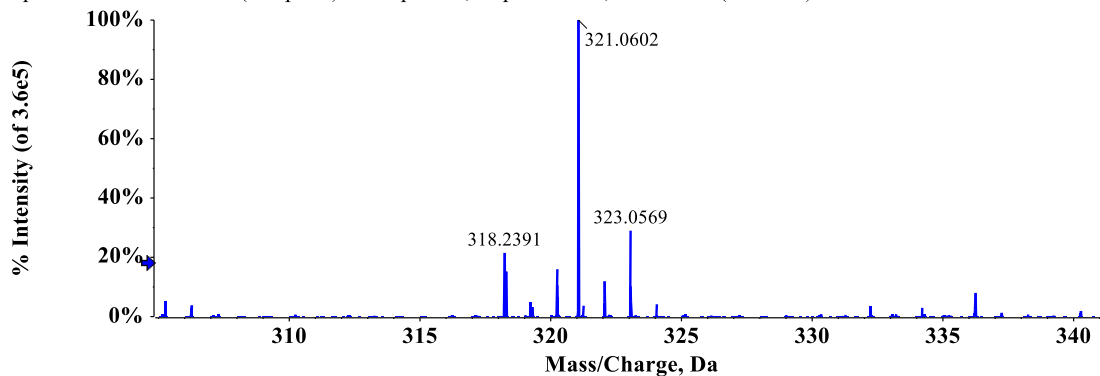


Figure 27. HRMS spectrum of target compound 6i

Compound 6j

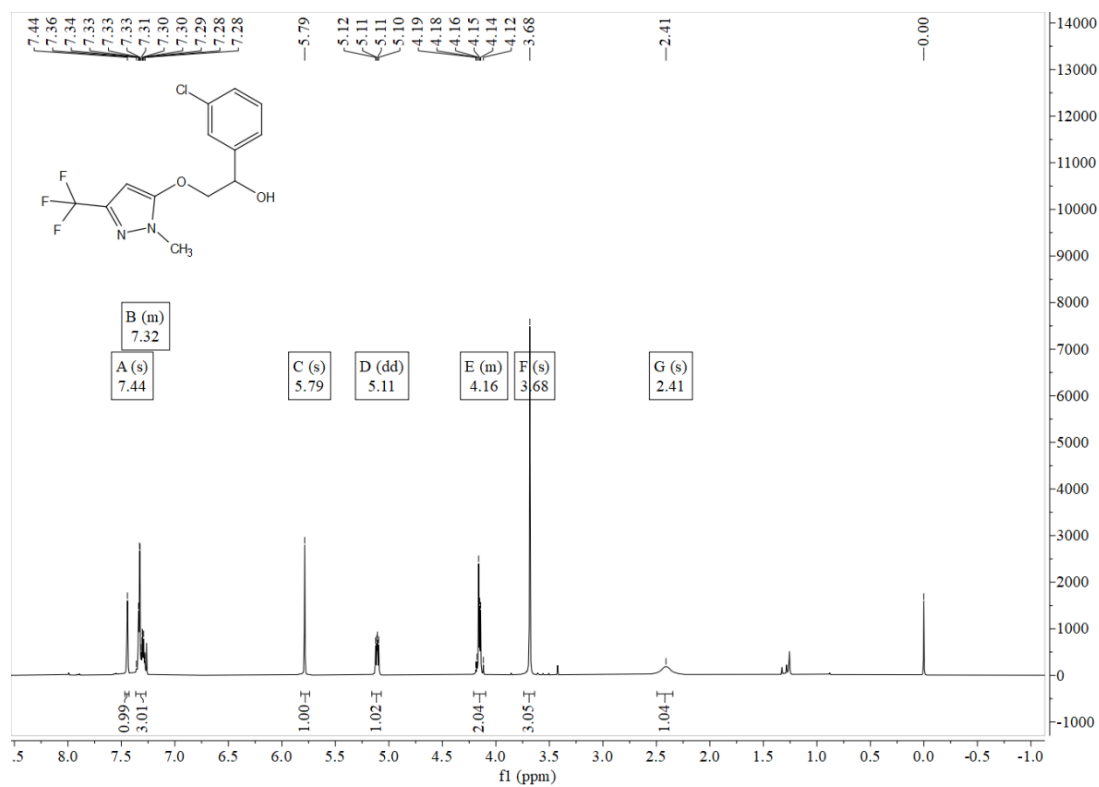


Figure 28. ¹H NMR spectrum of target compound 6j

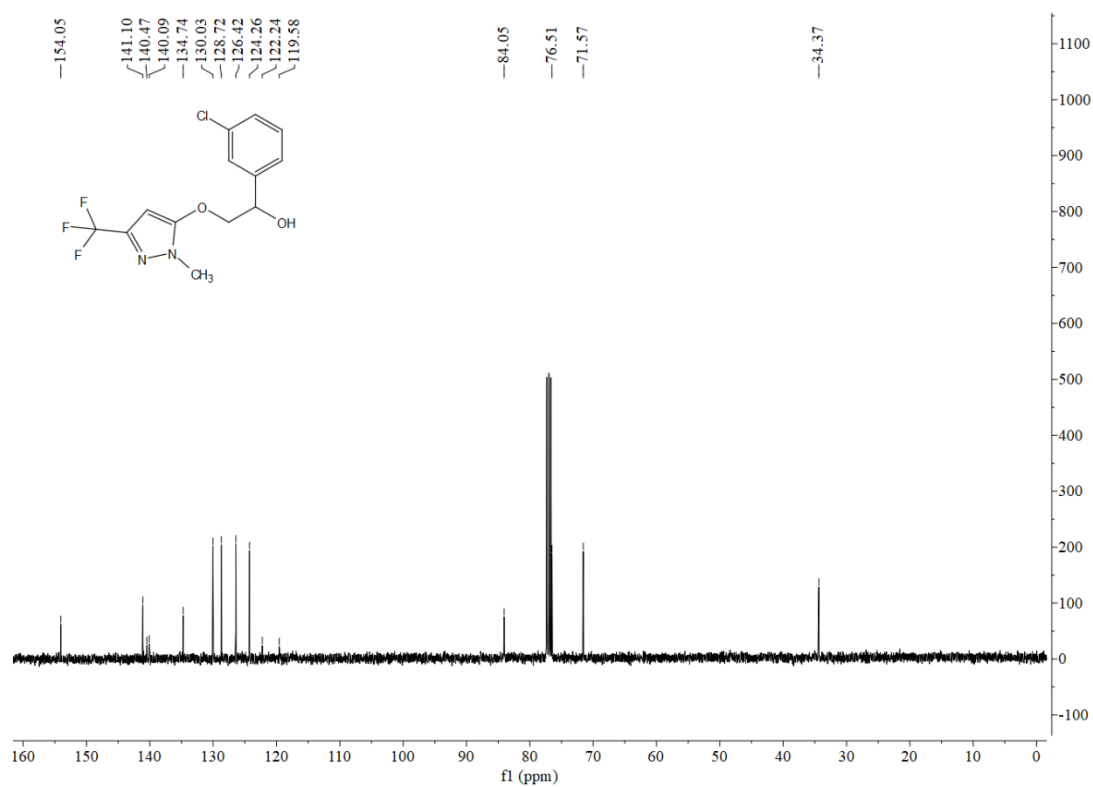


Figure 29. ¹³C NMR spectrum of target compound 6j

Spectrum from 6-7.wiff (sample 1) - Sample027, Experiment 1, +TOF MS (80 - 800) from 0.087 to 0.096 min

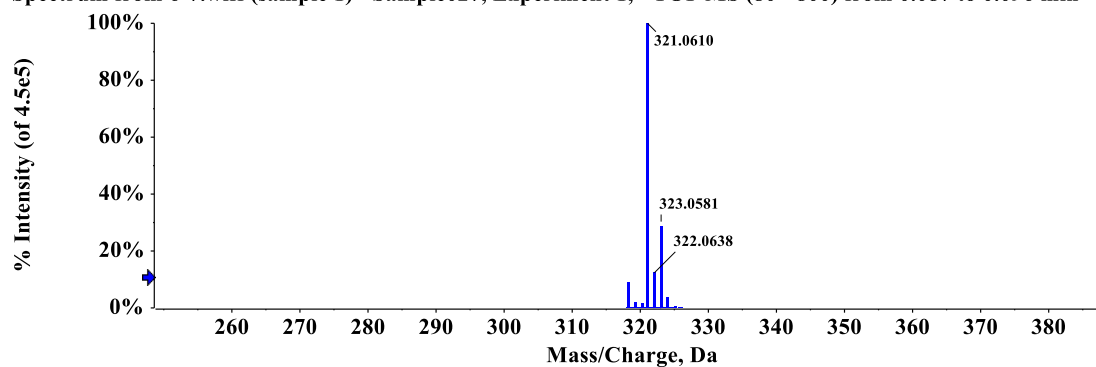


Figure 30. HRMS spectrum of target compound 6j

Compound 6k

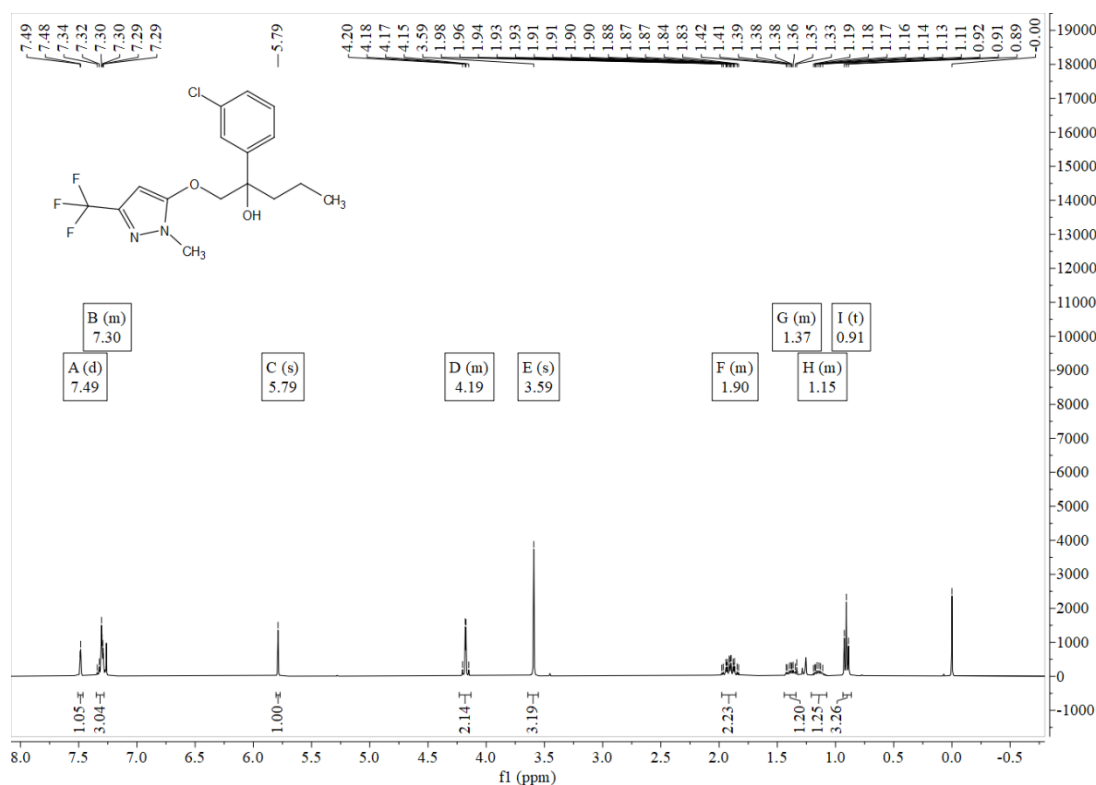


Figure 31. ¹H NMR spectrum of target compound 6k

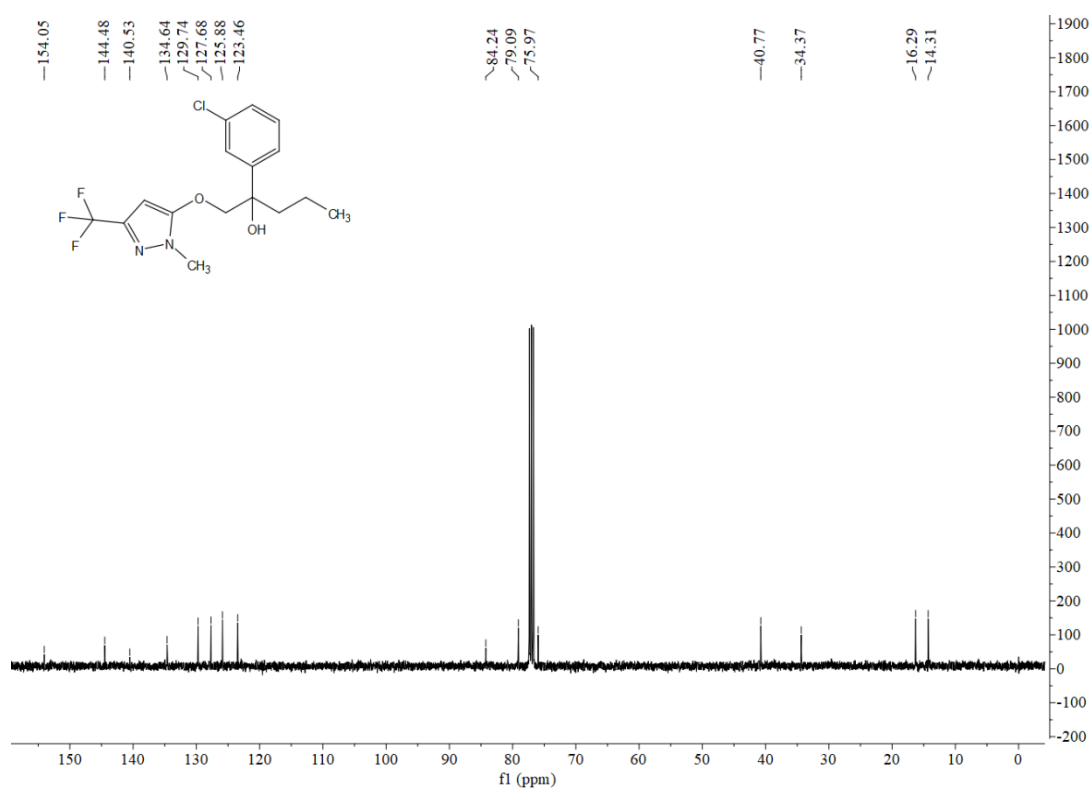


Figure 32. ¹³C NMR spectrum of target compound 6k

Spectrum from 6-6.wiff (sample 1) - Sample026, Experiment 1, +TOF MS (80 - 800) from 0.087 to 0.096 min

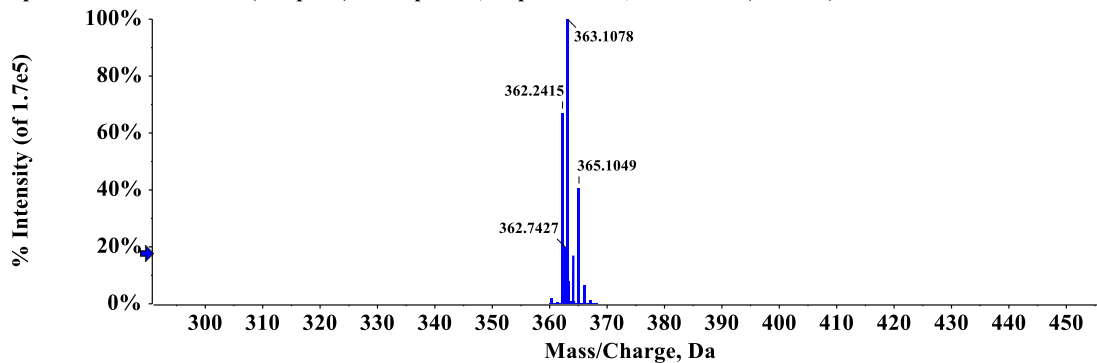


Figure 33. HRMS spectrum of target compound 6k

Compound 6l

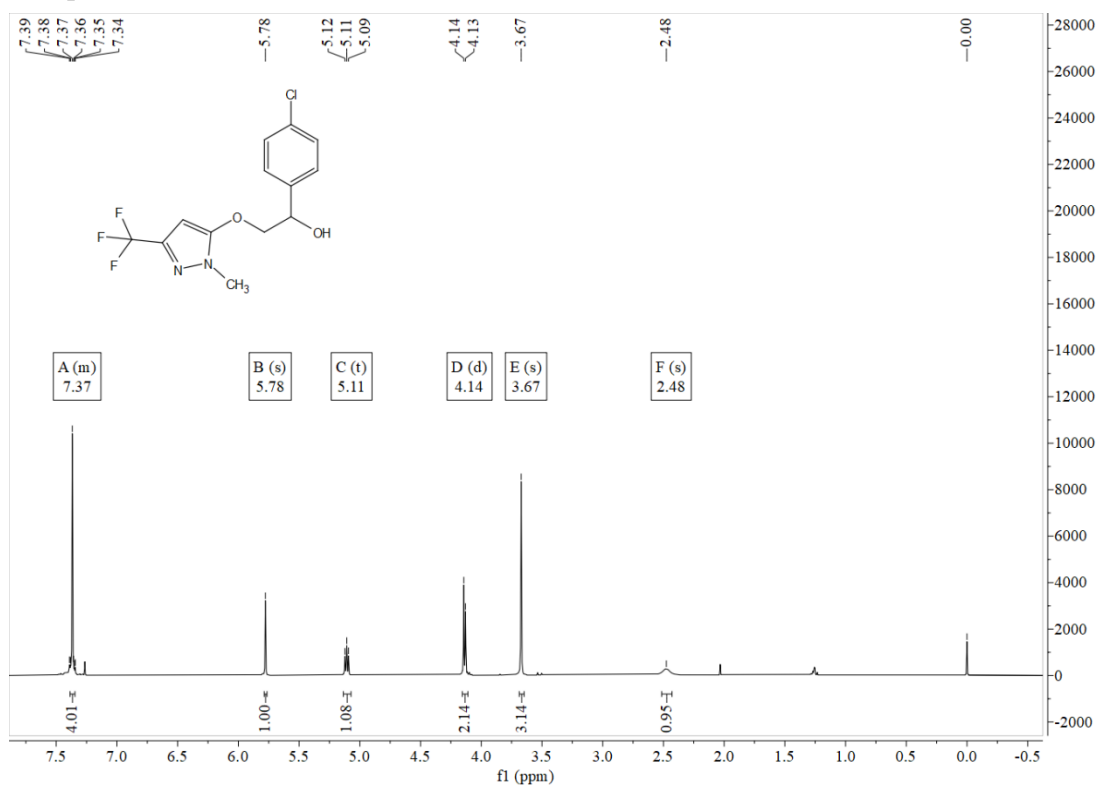


Figure 34. ¹H NMR spectrum of target compound 6l

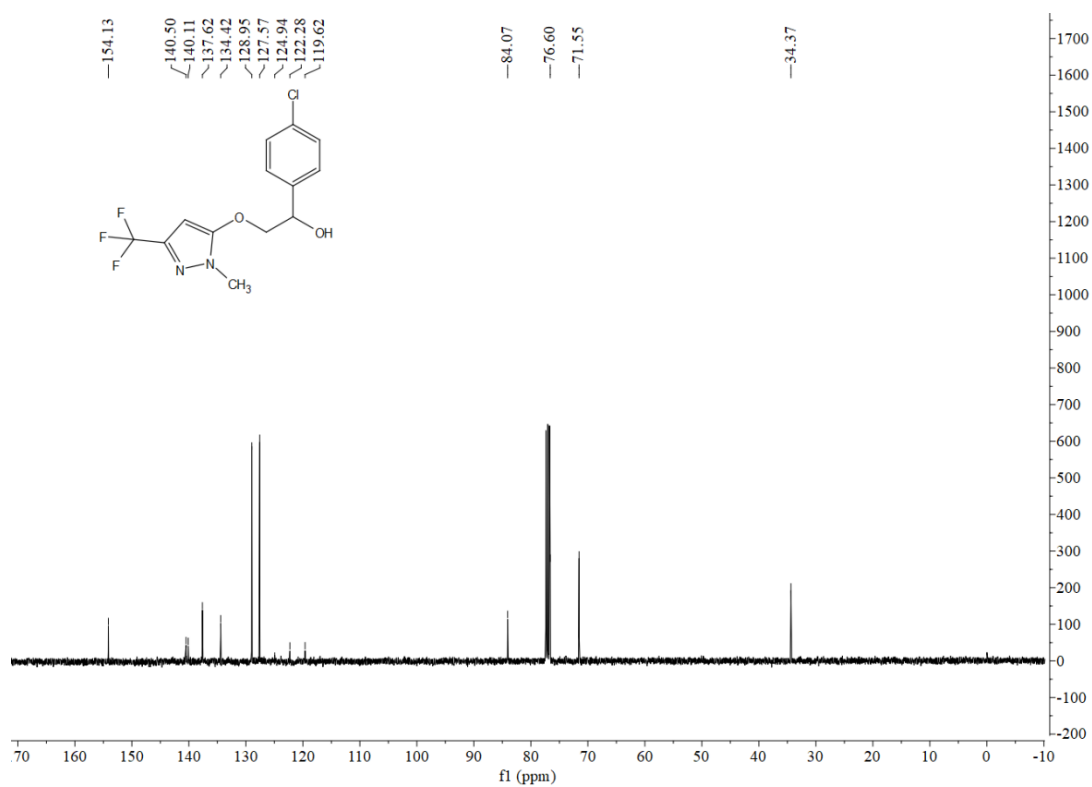


Figure 35. ¹³C NMR spectrum of target compound 6l

Spectrum from 5-3.wiff (sample 1) - Sample013, Ex...ent 1, +TOF MS (80 - 800) from 0.082 to 0.091 min

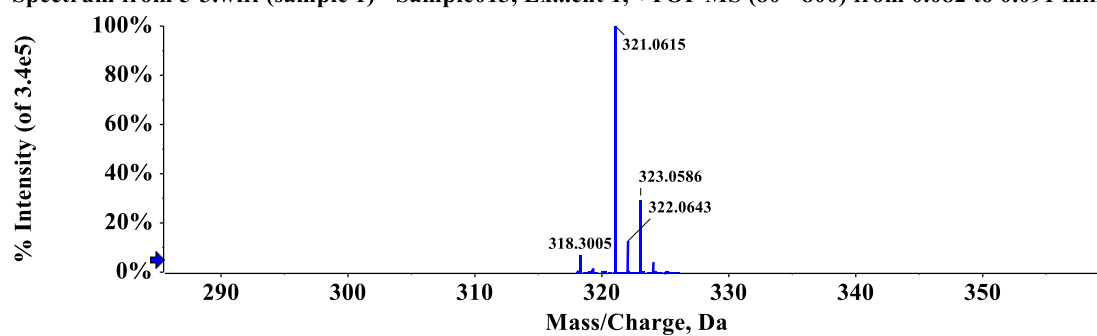


Figure 36. HRMS spectrum of target compound 6l

Compound 6m

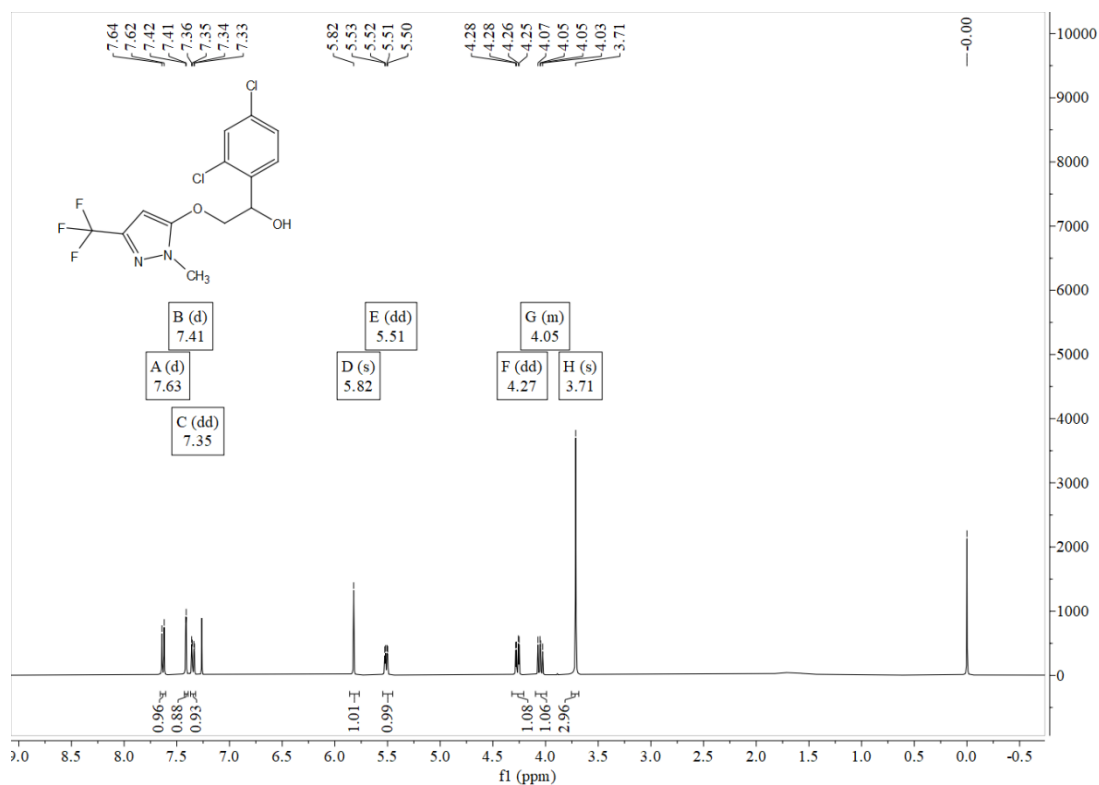


Figure 37. ¹H NMR spectrum of target compound 6m

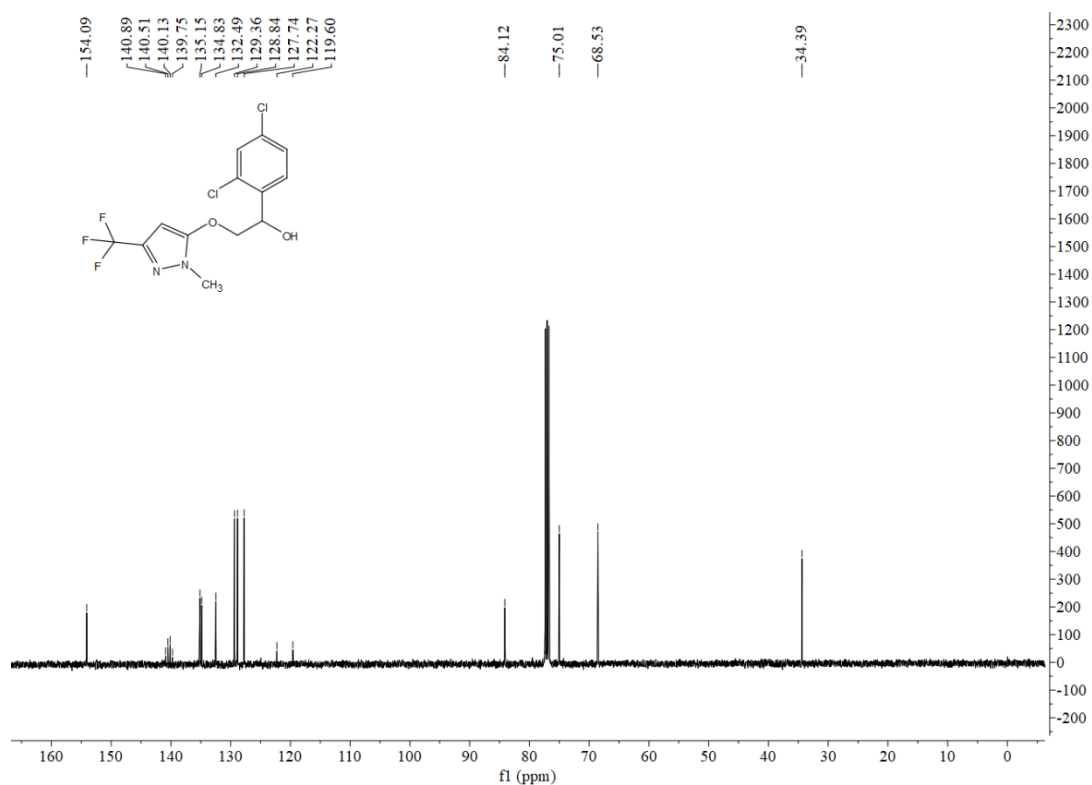


Figure 38. ¹³C NMR spectrum of target compound 6m

Spectrum from 5-1.wiff (sample 1) - Sample011, Ex...ent 1, +TOF MS (80 - 800) from 0.073 to 0.083 min

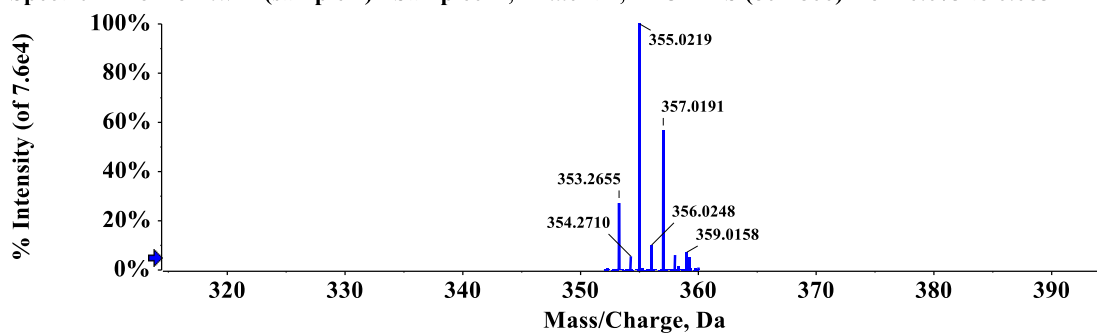


Figure 39. HRMS spectrum of target compound 6m

Compound 6n

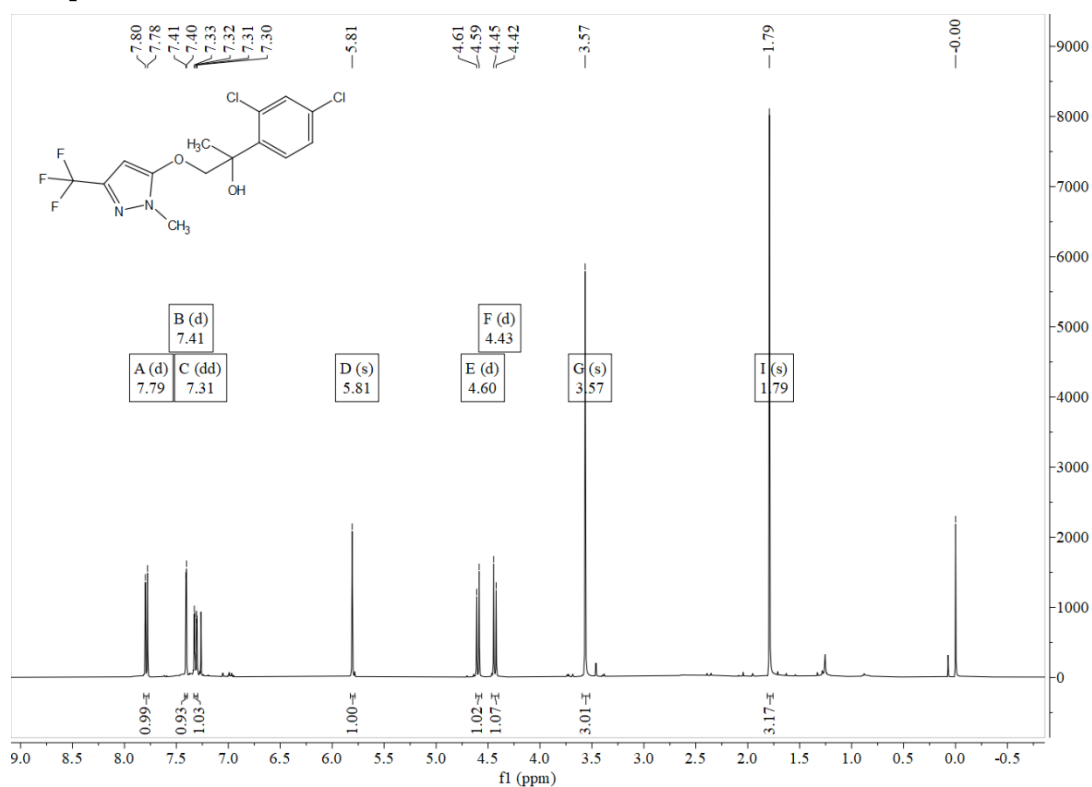


Figure 40. ¹H NMR spectrum of target compound 6n

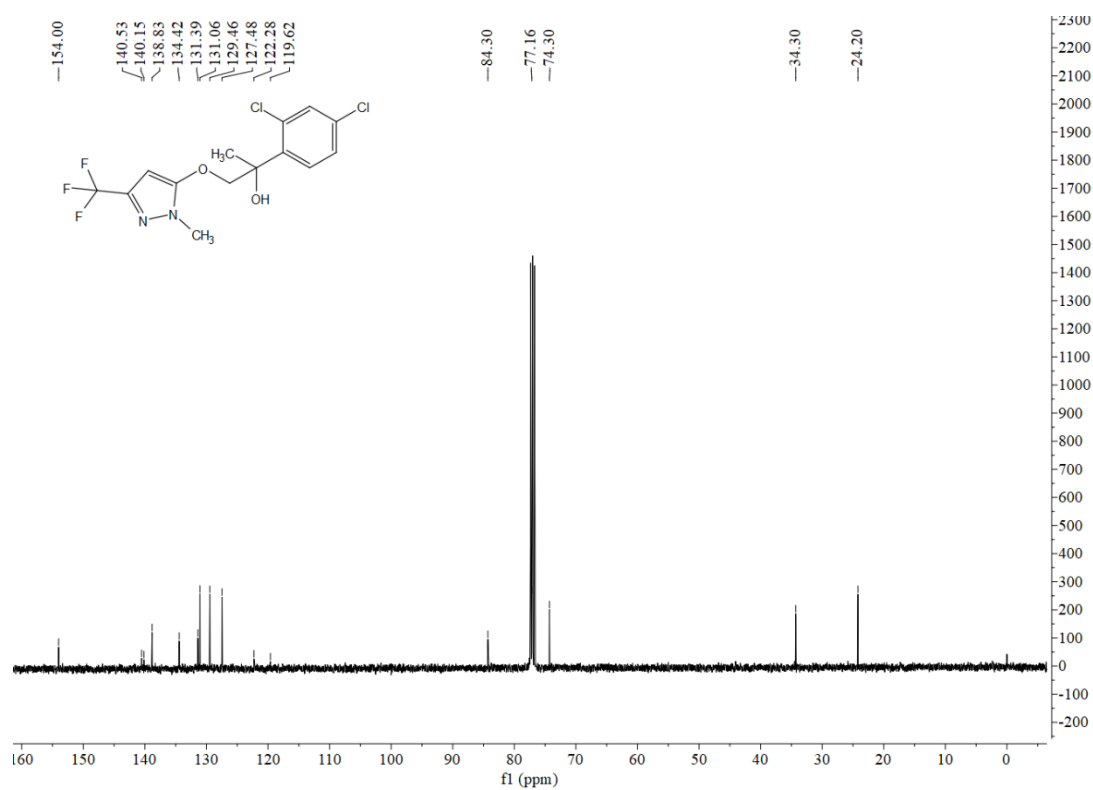


Figure 41. ¹³C NMR spectrum of target compound 6n

Spectrum from 5-2.wiff (sample 1) - Sample012, Ex...ent 1, +TOF MS (80 - 800) from 0.078 to 0.087 min

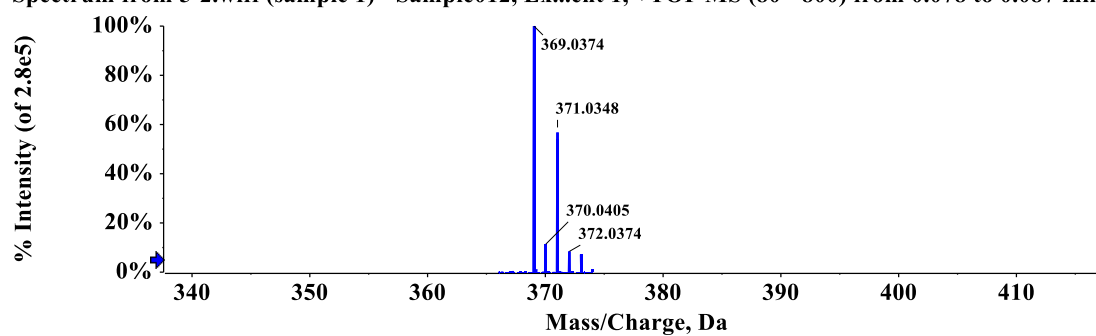


Figure 42. HRMS spectrum of target compound 6n

Compound 60

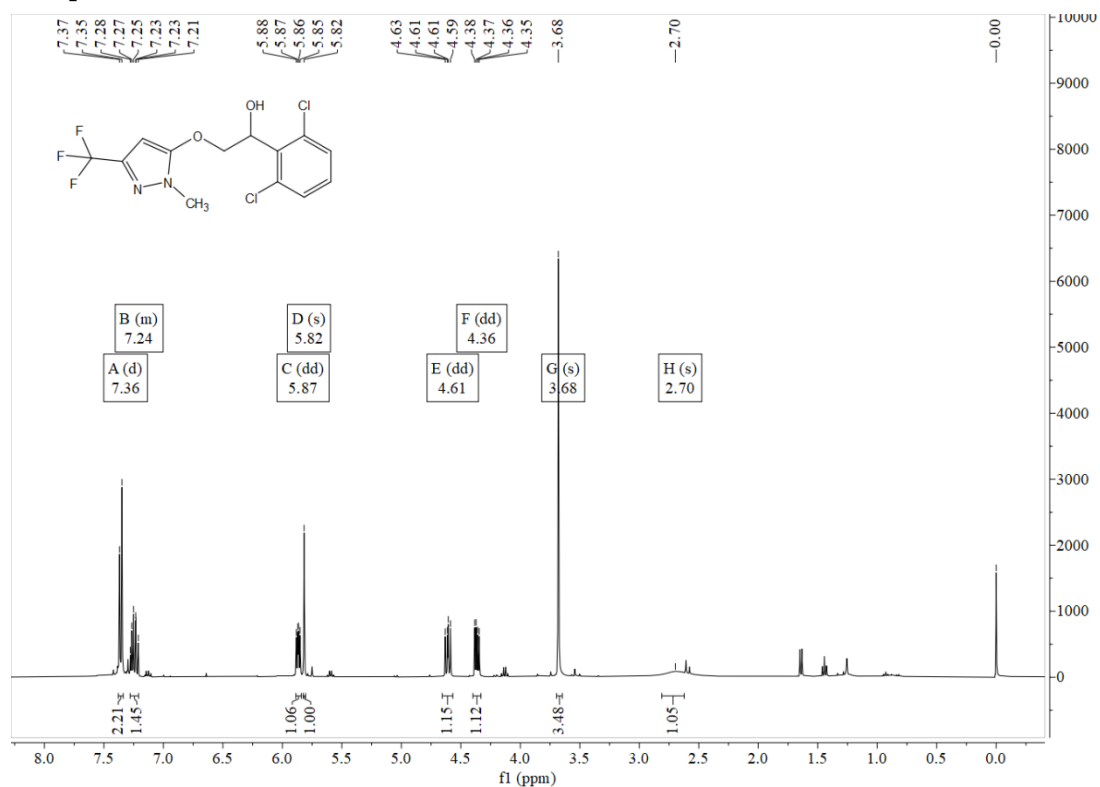


Figure 43. ¹H NMR spectrum of target compound 60

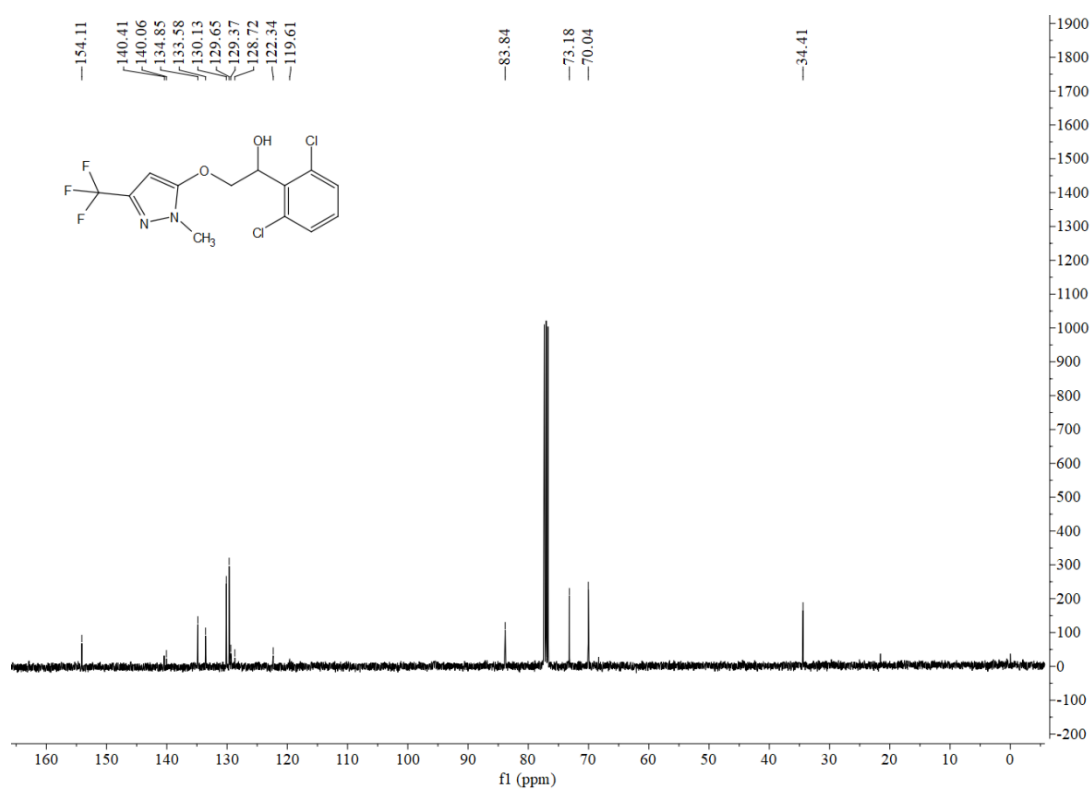


Figure 44. ¹³C NMR spectrum of target compound 60

Spectrum from 7-0.wiff (sample 1) - Sample030, Experiment 1, +TOF MS (80 - 800) from 0.097 min

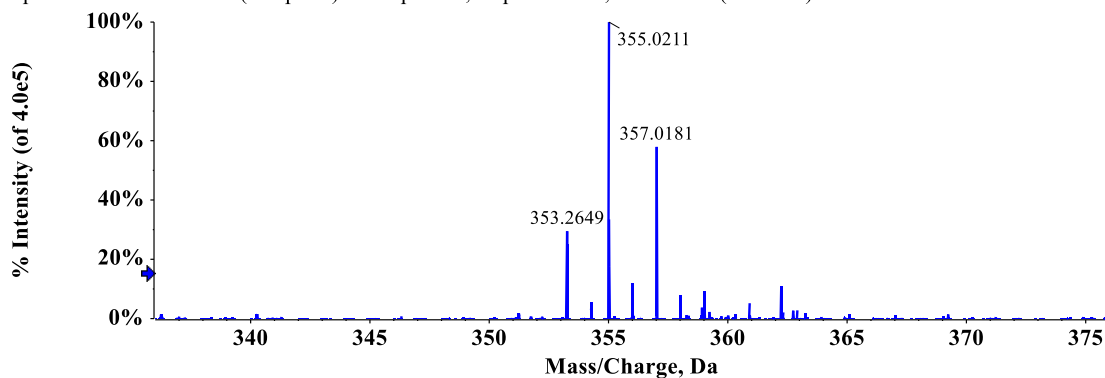


Figure 45. HRMS spectrum of target compound 6o

Compound 6p



Figure 46. ¹H NMR spectrum of target compound 6p

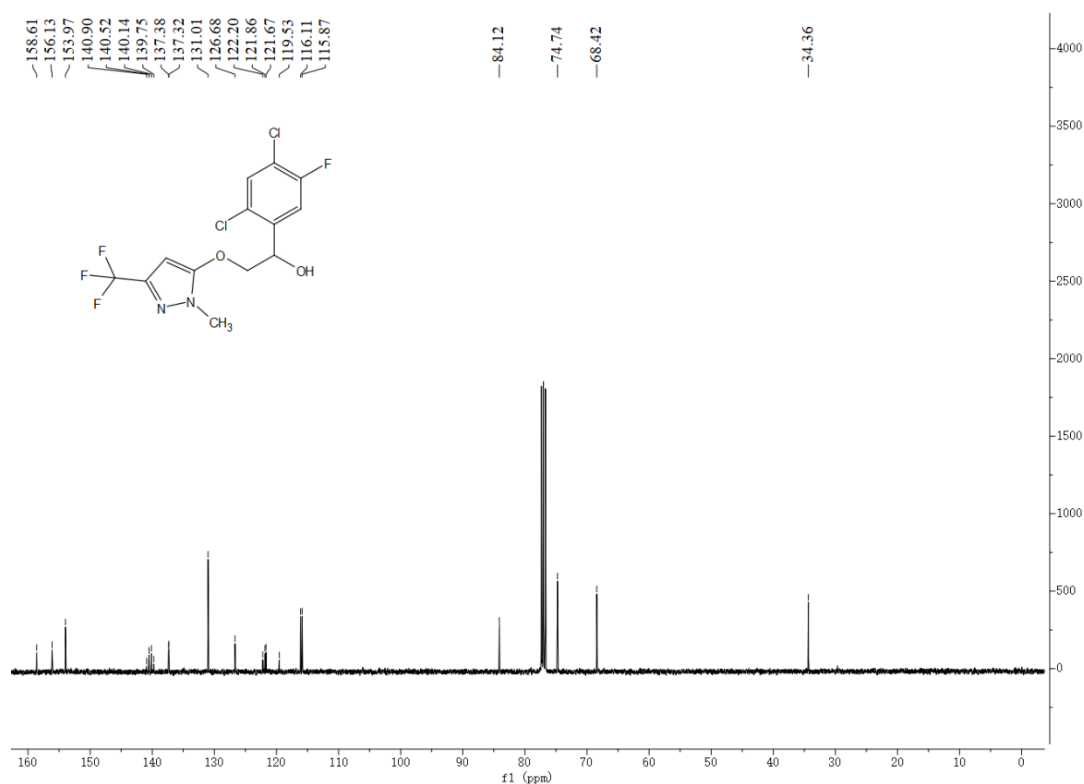


Figure 47. ¹³C NMR spectrum of target compound 6p

Spectrum from 7-7.wiff (sample 1) - Sample037, Experiment 1, +TOF MS (80 - 800) from 0.087 min

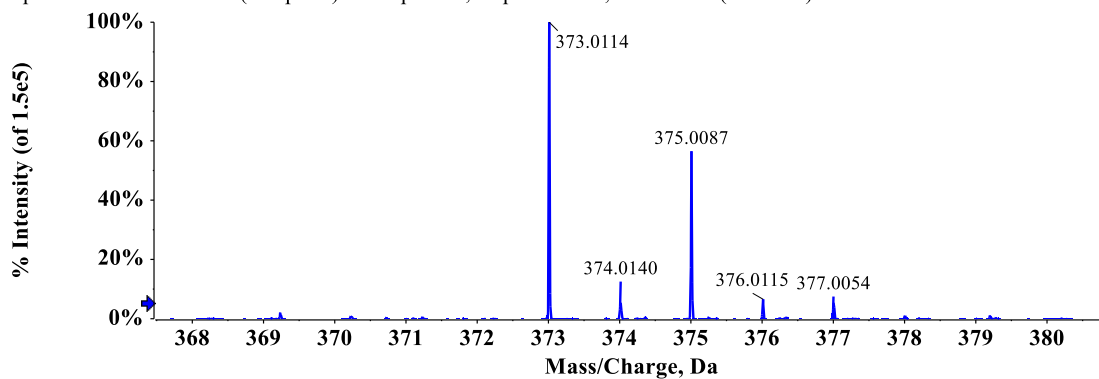


Figure 48. HRMS spectrum of target compound 6p

Compound 6q

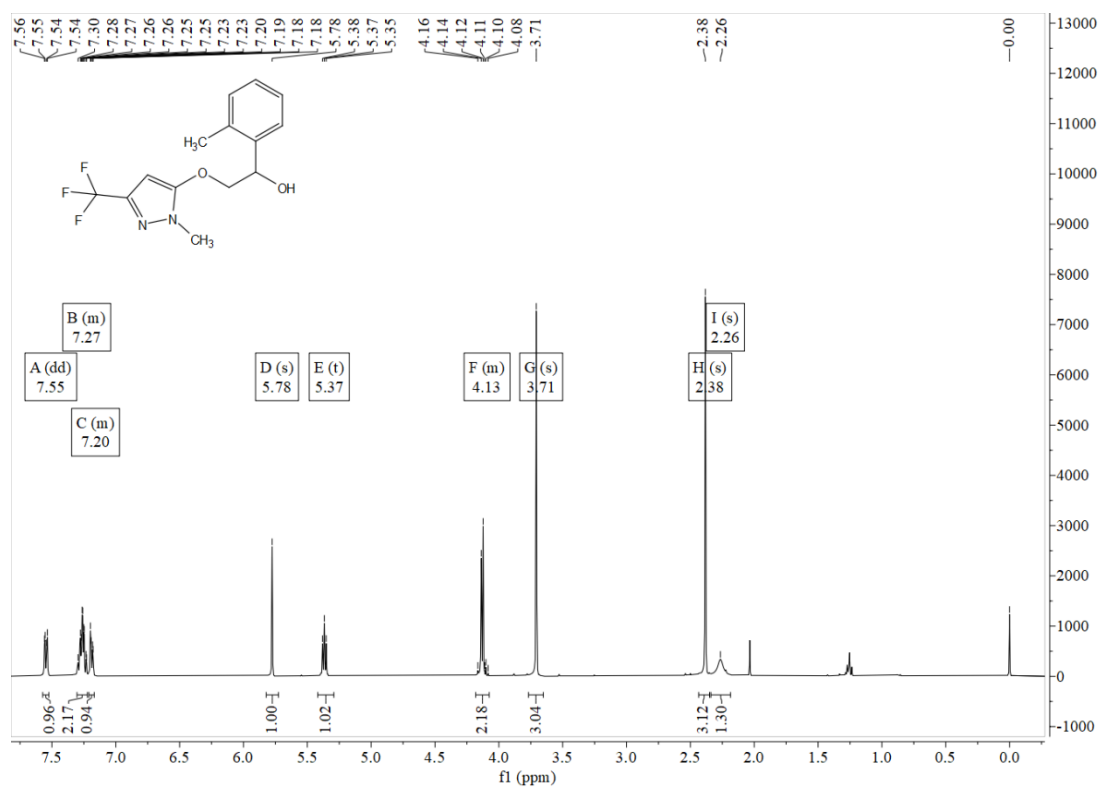


Figure 49. ¹H NMR spectrum of target compound 6q

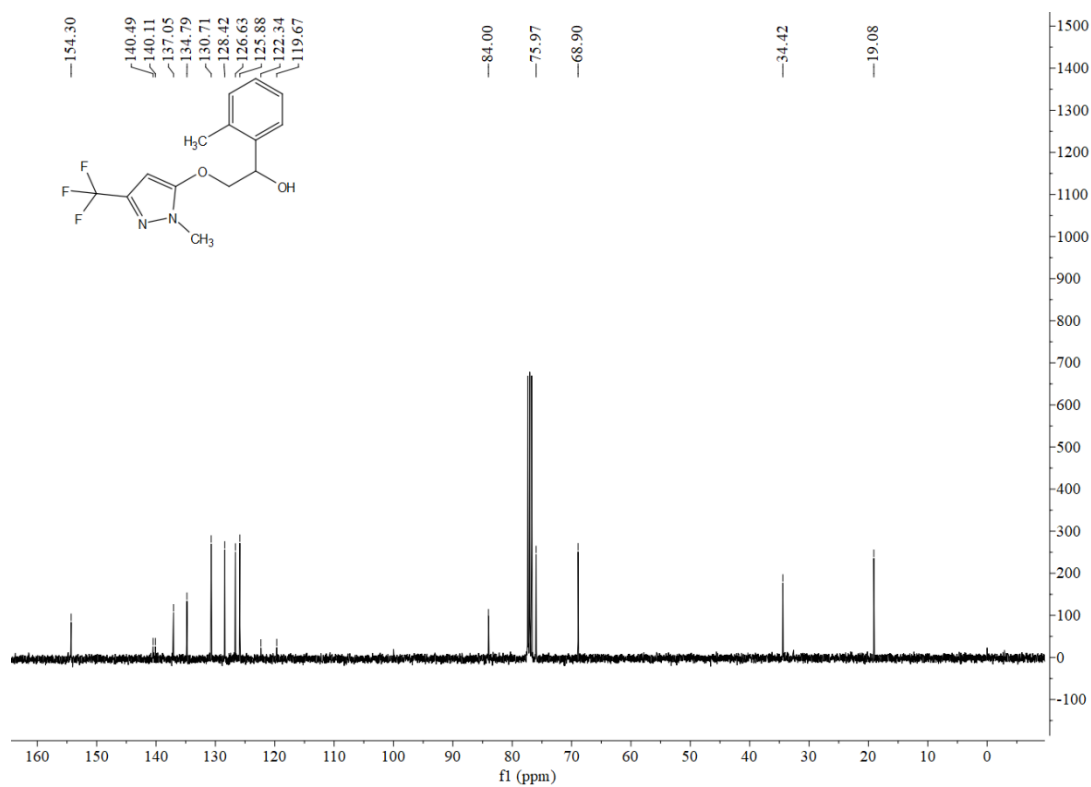


Figure 50. ¹³C NMR spectrum of target compound 6q

Spectrum from 6-3.wiff (sample 1) - Sample023, Ex...ent 1, +TOF MS (80 - 800) from 0.087 to 0.096 min

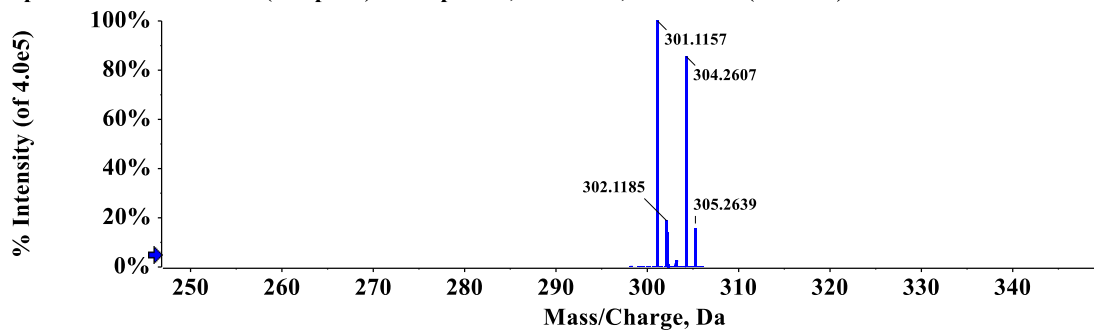


Figure 51. HRMS spectrum of target compound 6q

Compound 6r

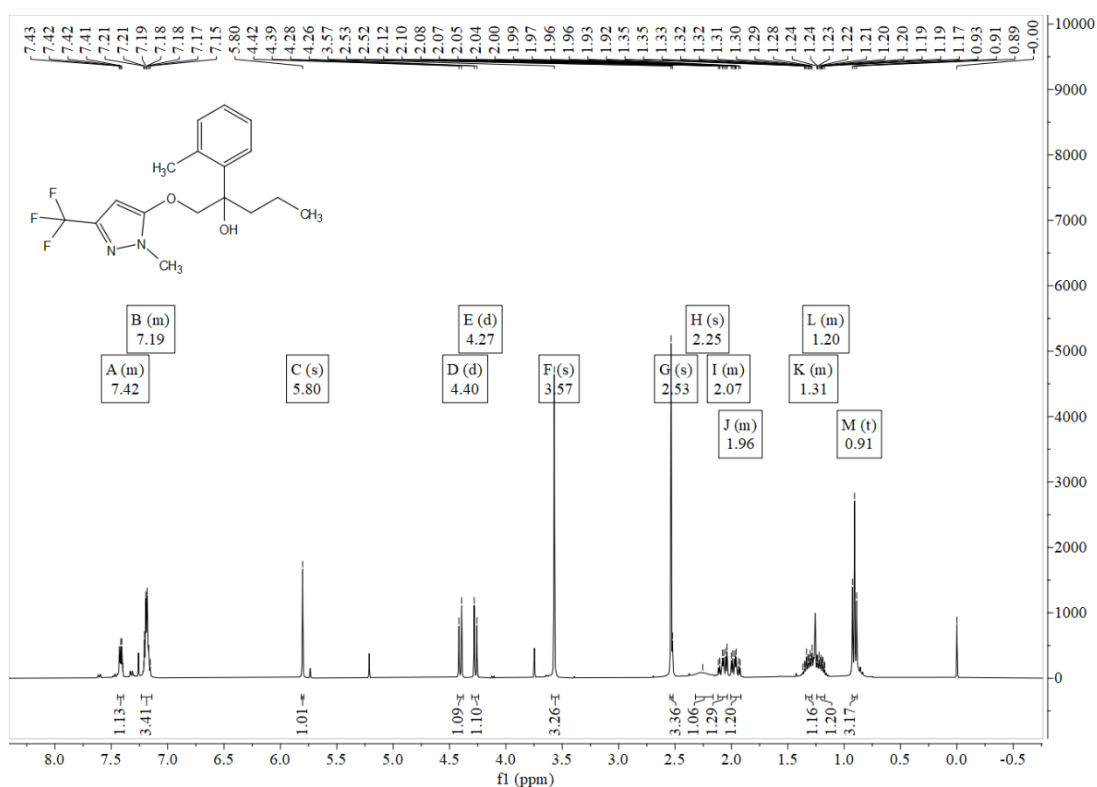


Figure 52. ^1H NMR spectrum of target compound 6r

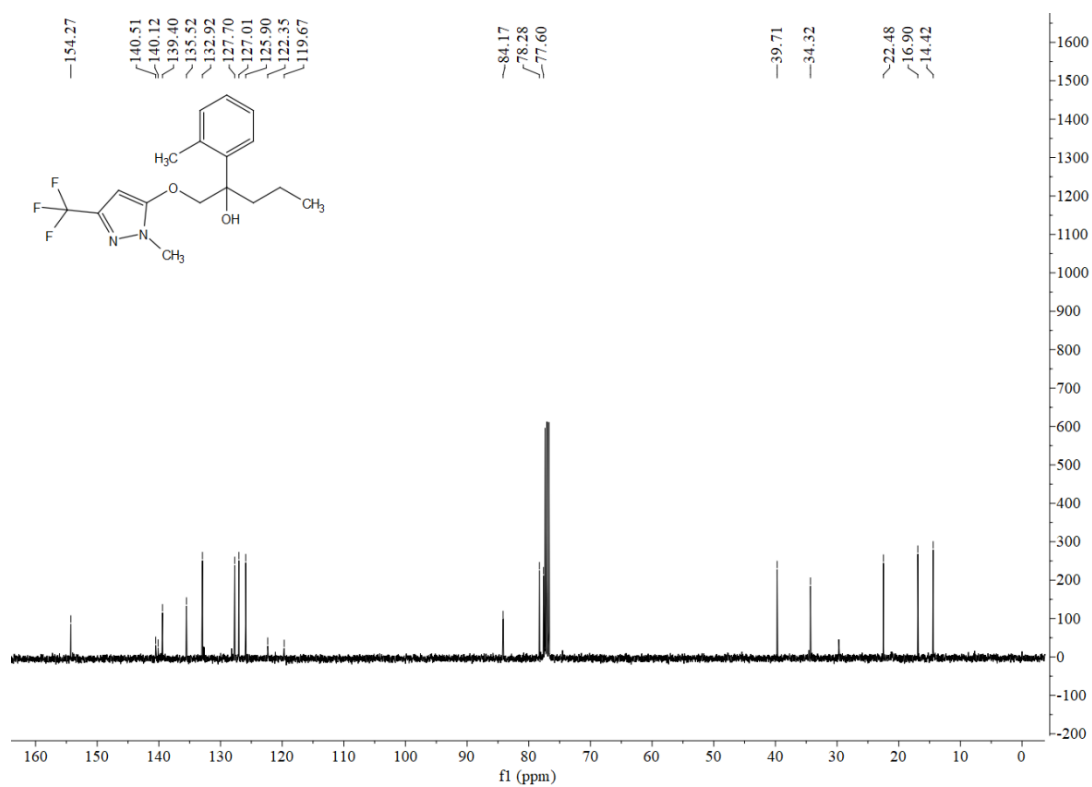


Figure 53. ¹³C NMR spectrum of target compound 6r

Spectrum from 6-2.wiff (sample 1) - Sample022, Ex...ent 1, +TOF MS (80 - 800) from 0.077 to 0.086 min

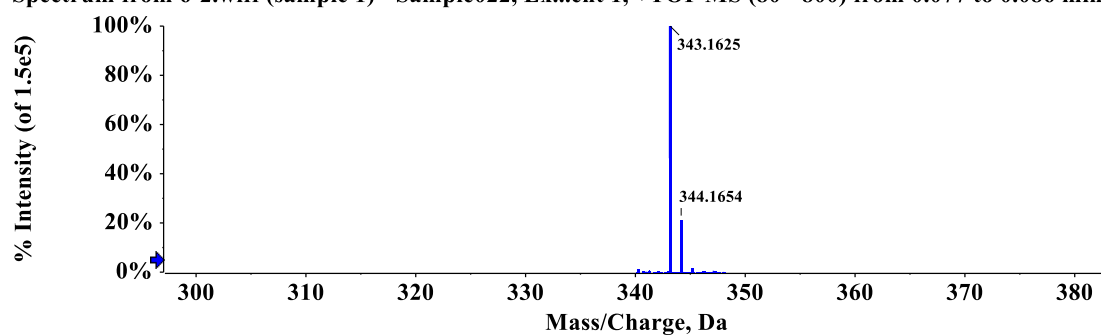


Figure 54. HRMS spectrum of target compound 6r

Compound 6s

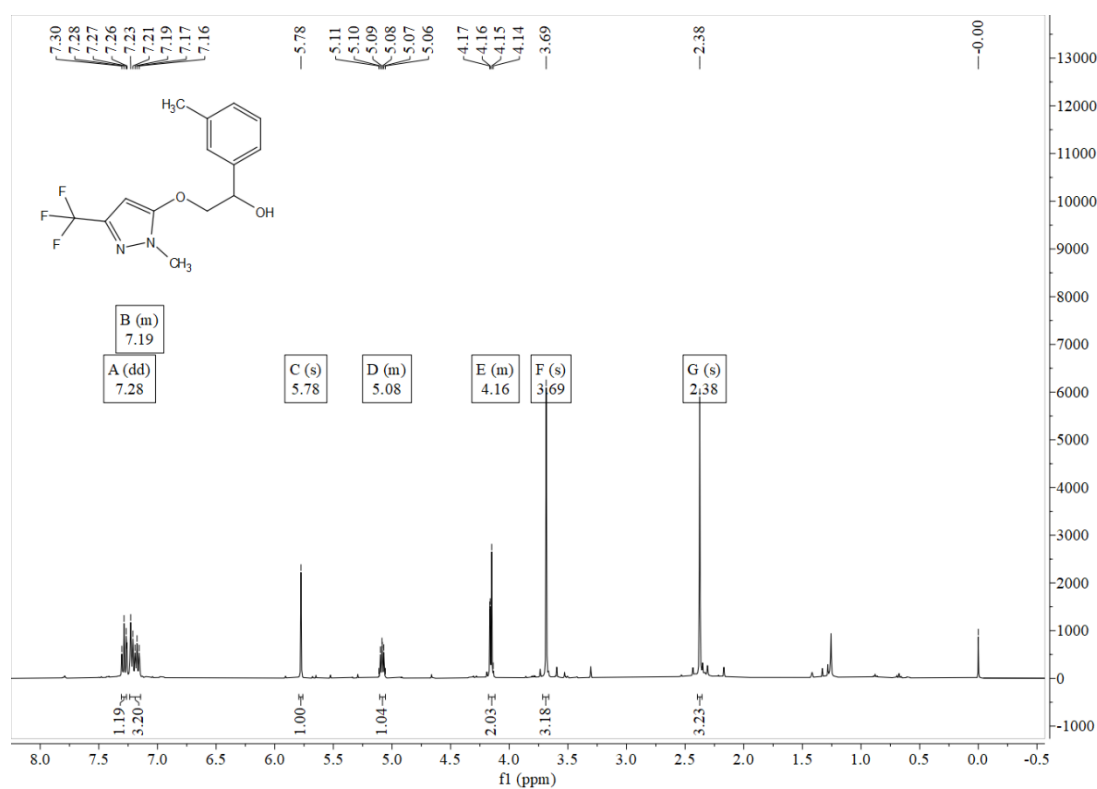


Figure 55. ¹H NMR spectrum of target compound 6s

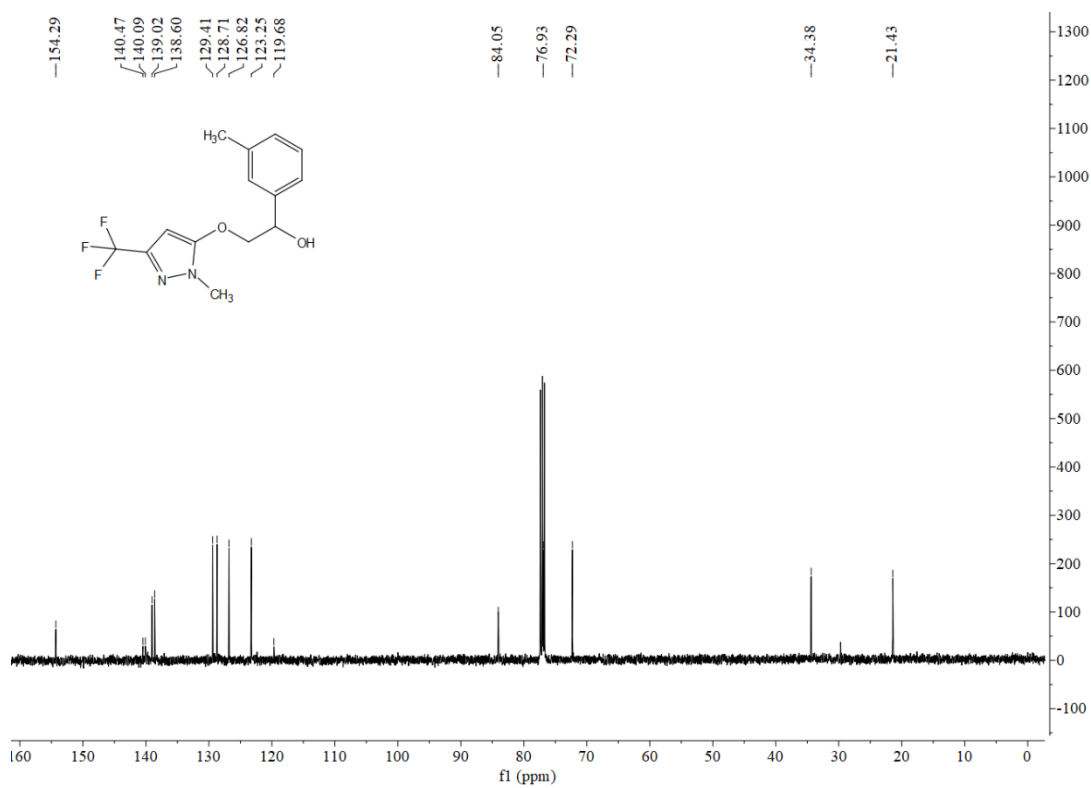


Figure 56. ¹³C NMR spectrum of target compound 6s

Spectrum from 6-8.wiff (sample 1) - Sample028, Ex...ent 1, +TOF MS (80 - 800) from 0.082 to 0.091 min

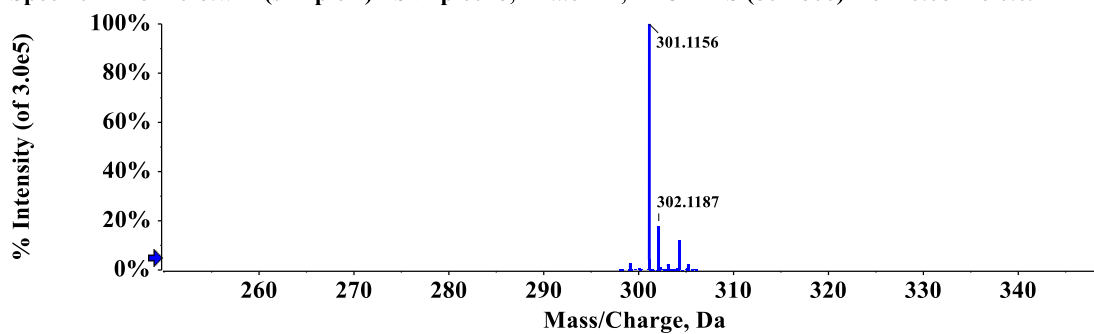


Figure 57. HRMS spectrum of target compound 6s

Compound 6t

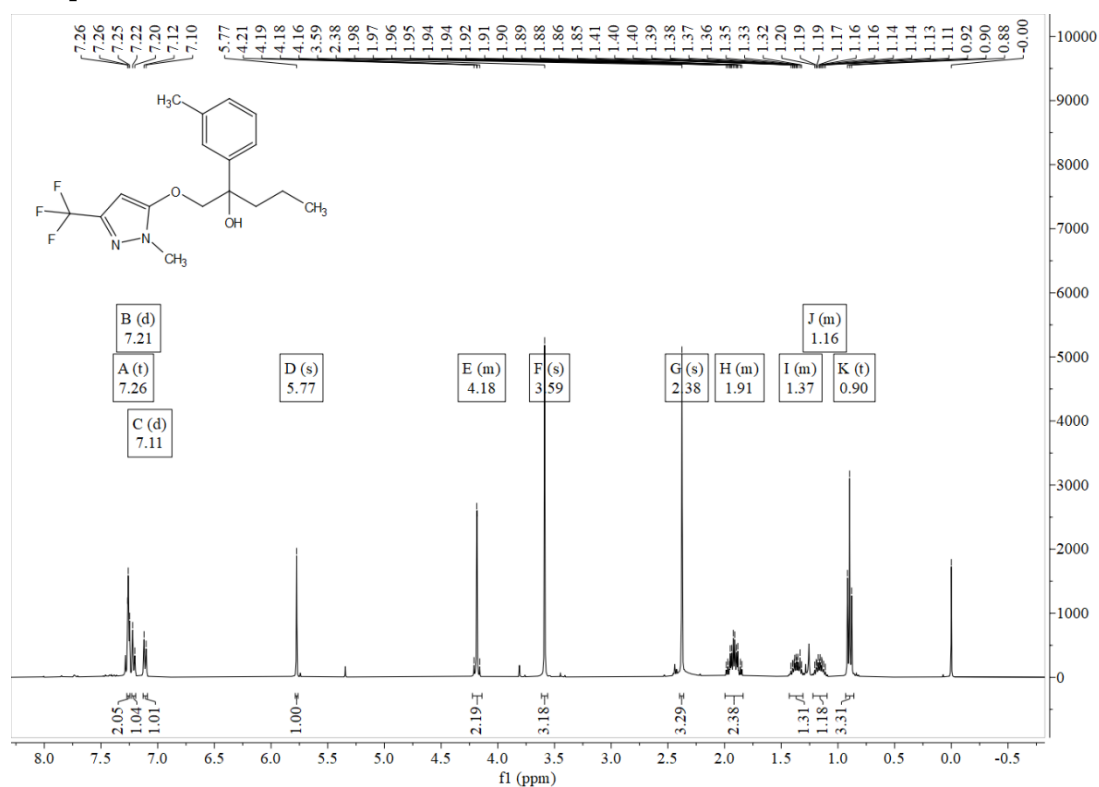


Figure 58. ¹H NMR spectrum of target compound 6t

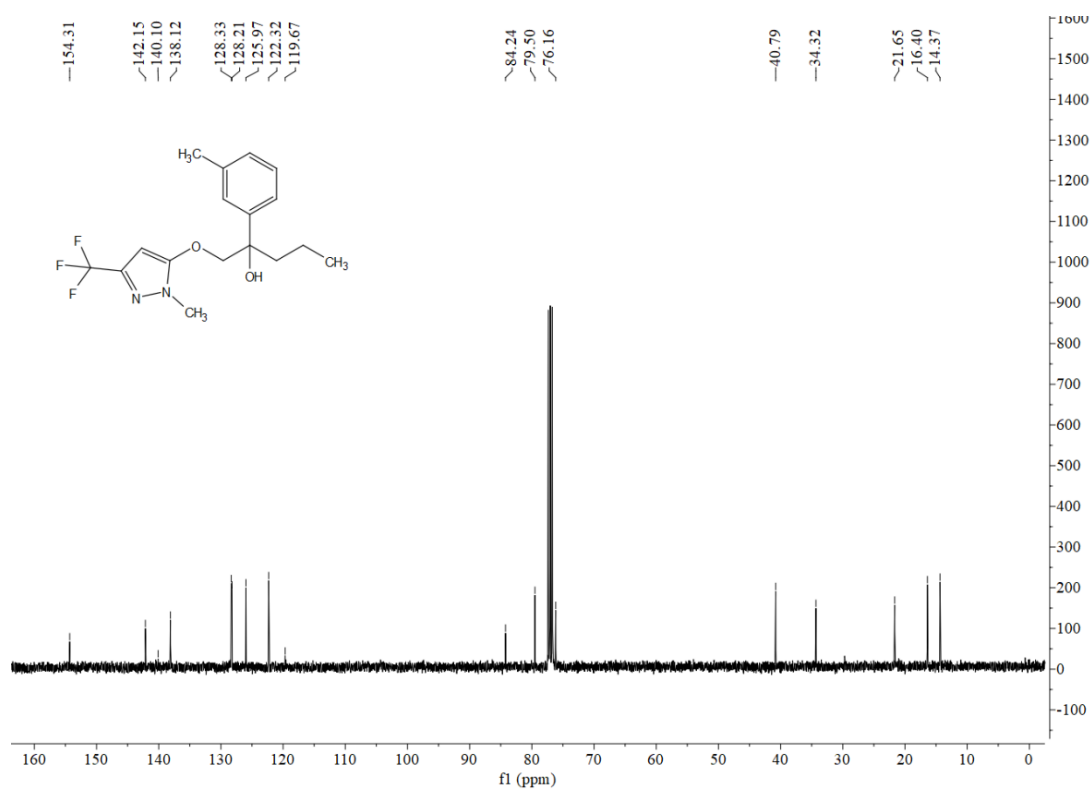


Figure 59. ¹³C NMR spectrum of target compound 6t

Spectrum from 6-9.wiff (sample 1) - Sample029, Ex...ent 1, +TOF MS (80 - 800) from 0.087 to 0.096 min

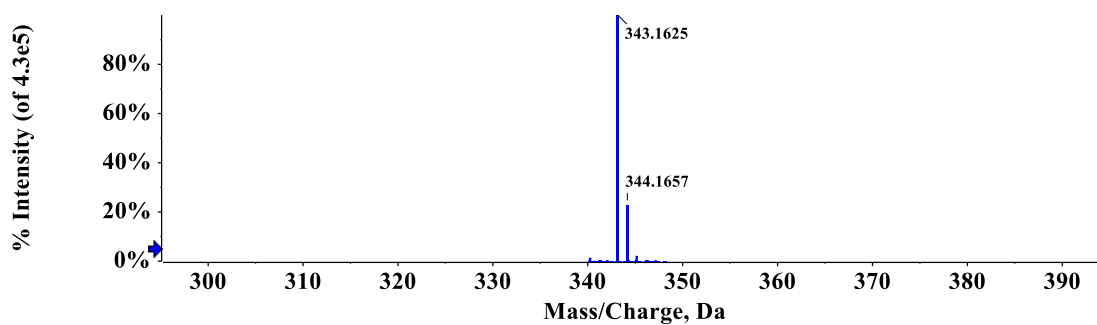


Figure 60. HRMS spectrum of target compound 6t

Compound 6u

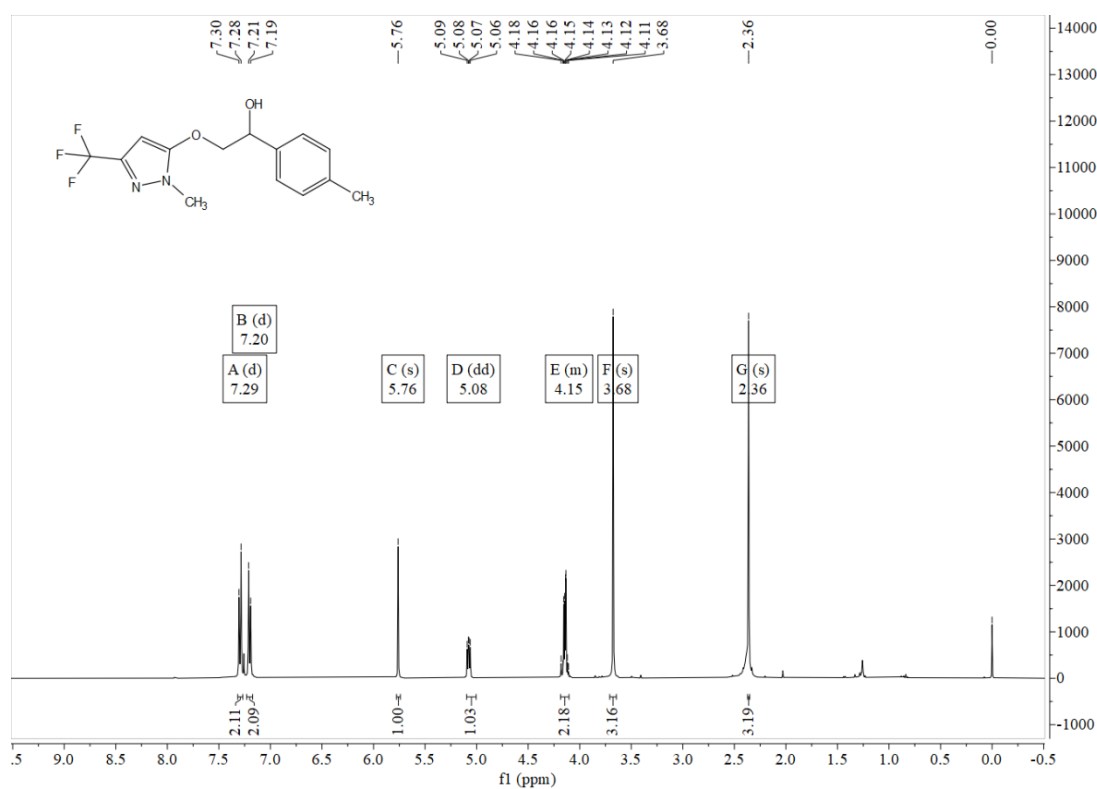


Figure 61. ¹H NMR spectrum of target compound 6u

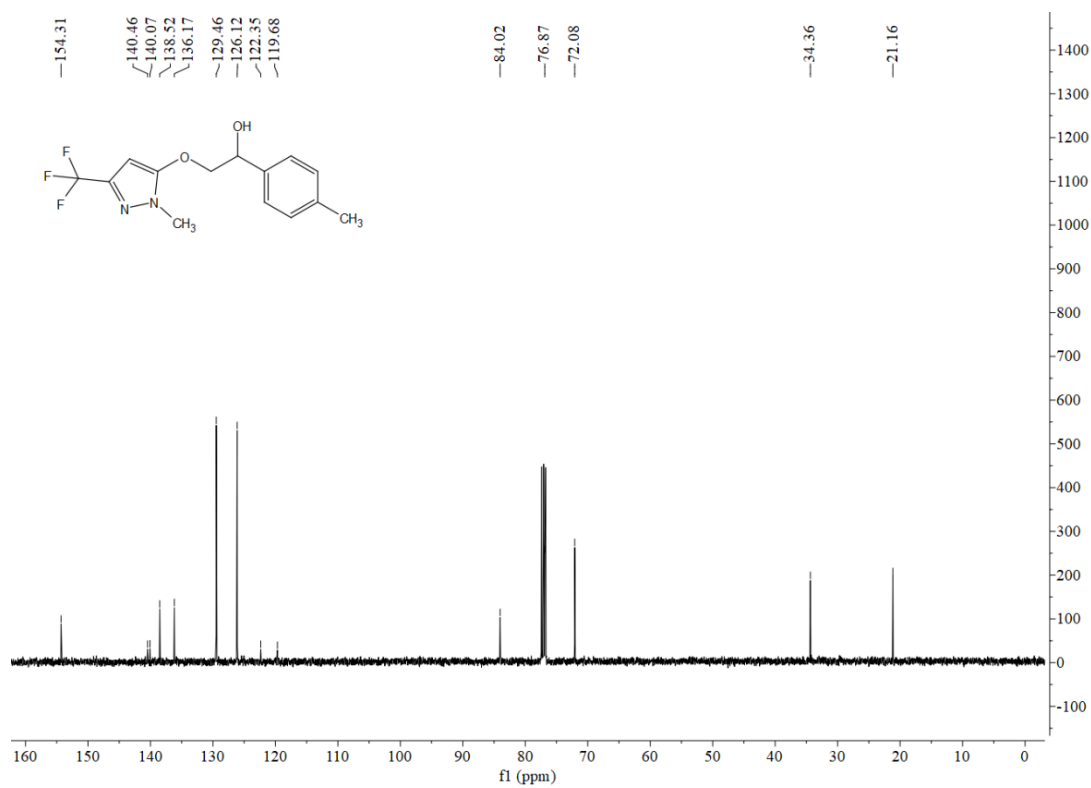


Figure 62. ¹³C NMR spectrum of target compound 6u

Spectrum from 5-5.wiff (sample 1) - Sample015, Ex...ent 1, +TOF MS (80 - 800) from 0.077 to 0.086 min

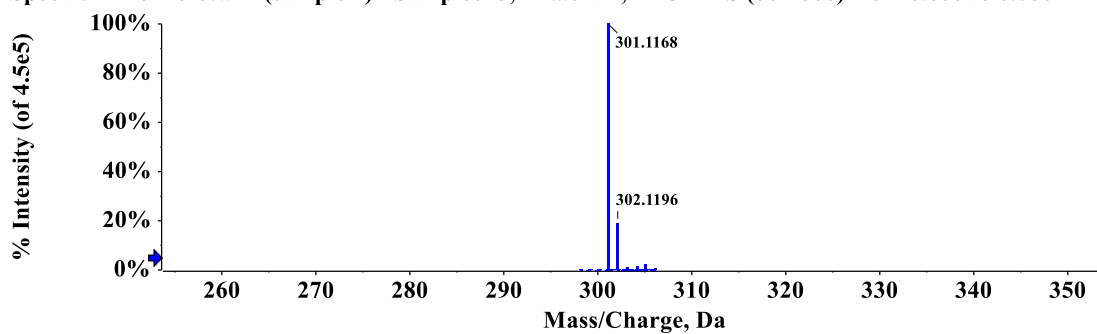


Figure 63. HRMS spectrum of target compound 6u

Compound 6v

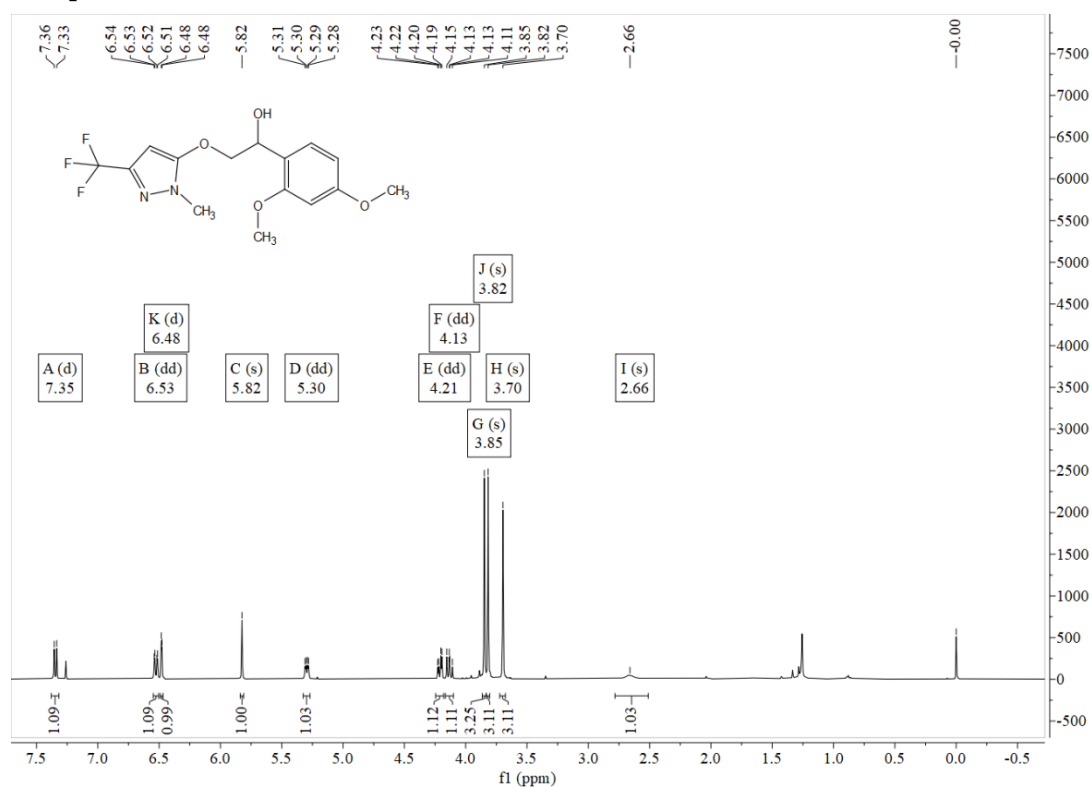


Figure 64. ¹H NMR spectrum of target compound 6v

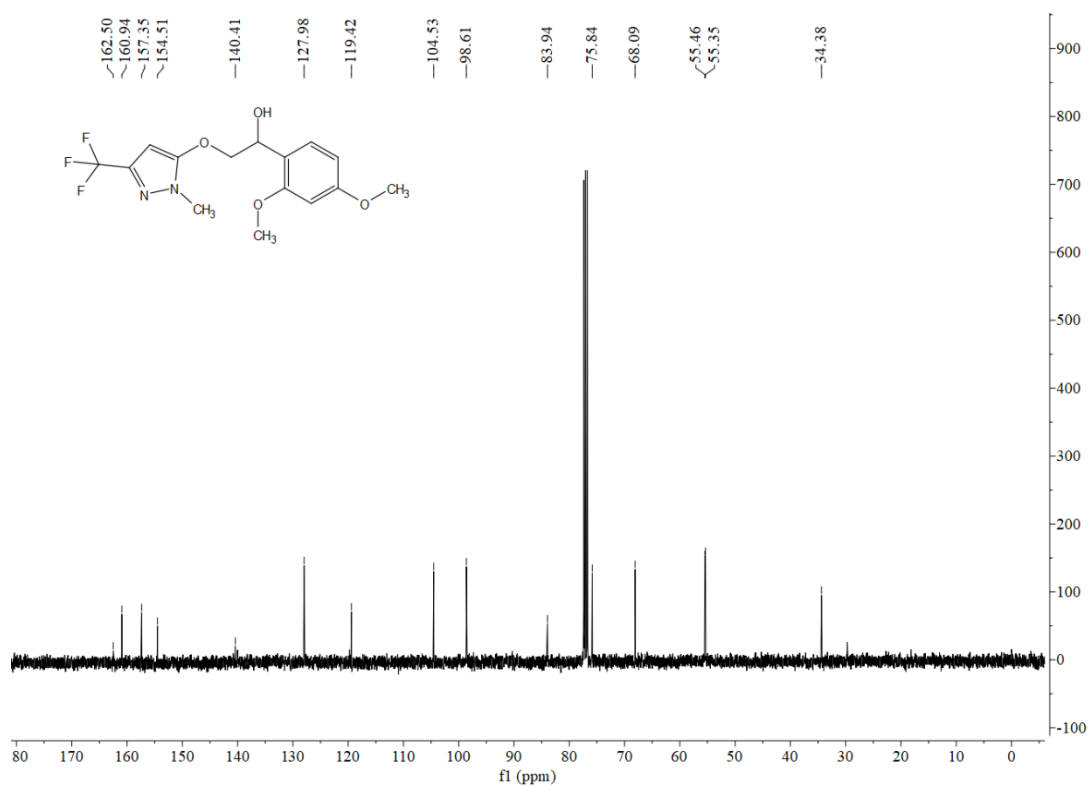


Figure 65. ¹³C NMR spectrum of target compound 6v

Spectrum from 6-0.wiff (sample 1) - Sample020, Ex...ent 1, +TOF MS (80 - 800) from 0.078 to 0.087 min

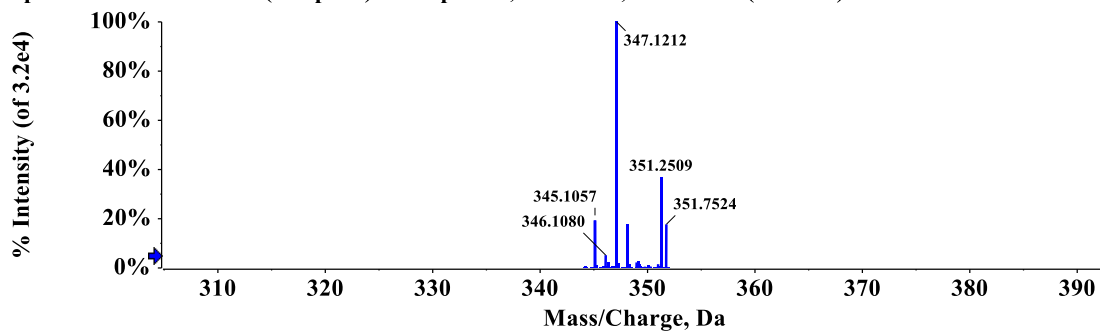


Figure 66. HRMS spectrum of target compound 6v

Compound 6w

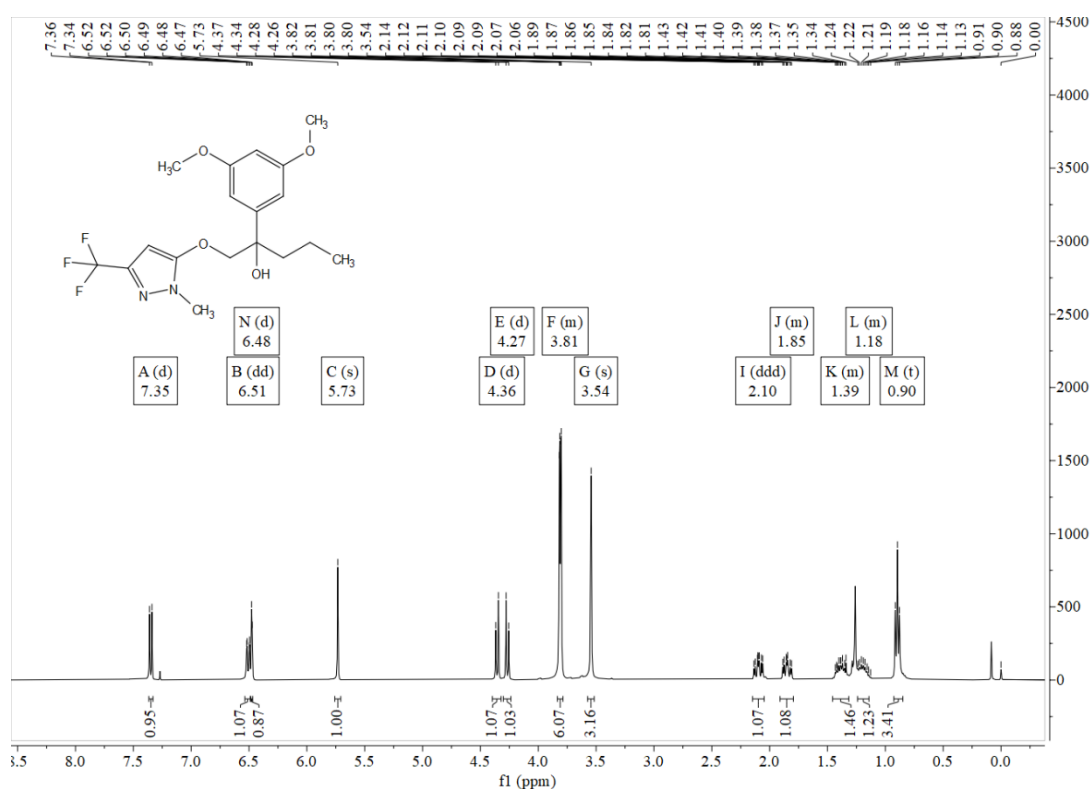


Figure 67. ¹H NMR spectrum of target compound 6w

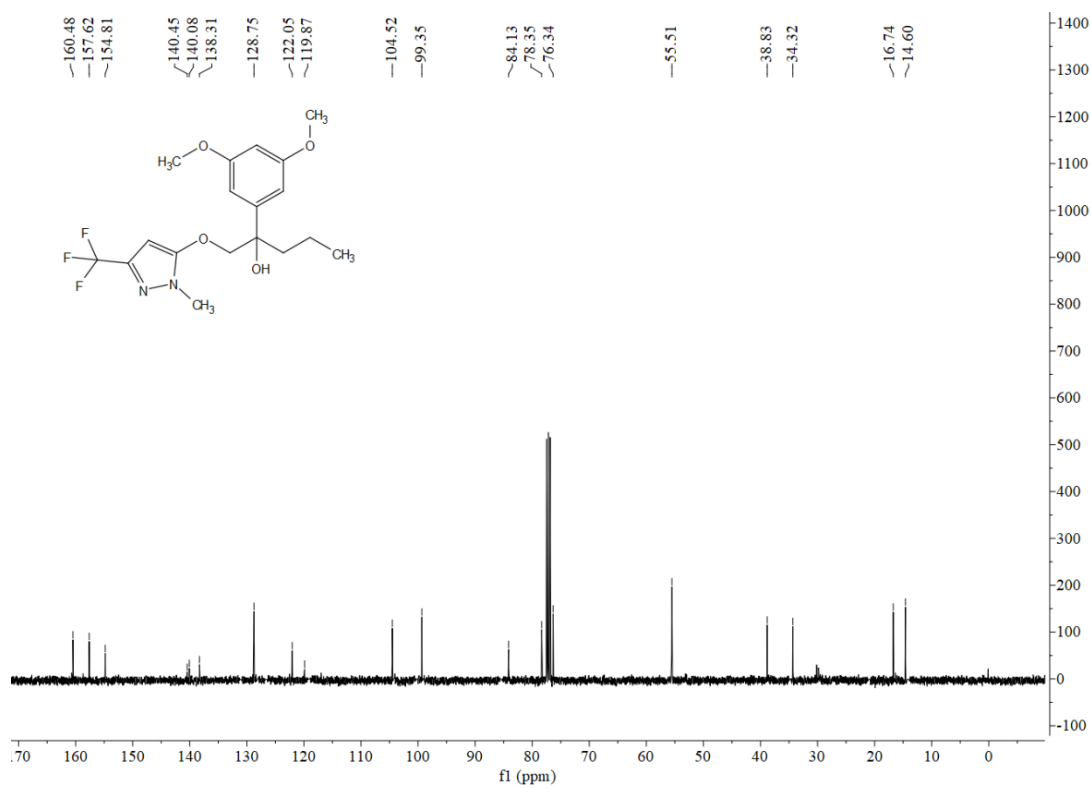


Figure 68. ¹³C NMR spectrum of target compound 6w

Spectrum from 5-9.wiff (sample 1) - Sample019, Ex...ent 1, +TOF MS (80 - 800) from 0.087 to 0.096 min

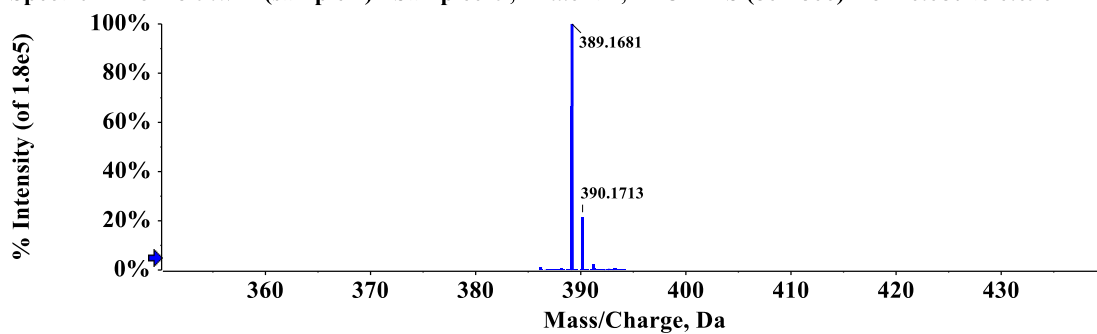


Figure 69. HRMS spectrum of target compound 6w

Compound 6x

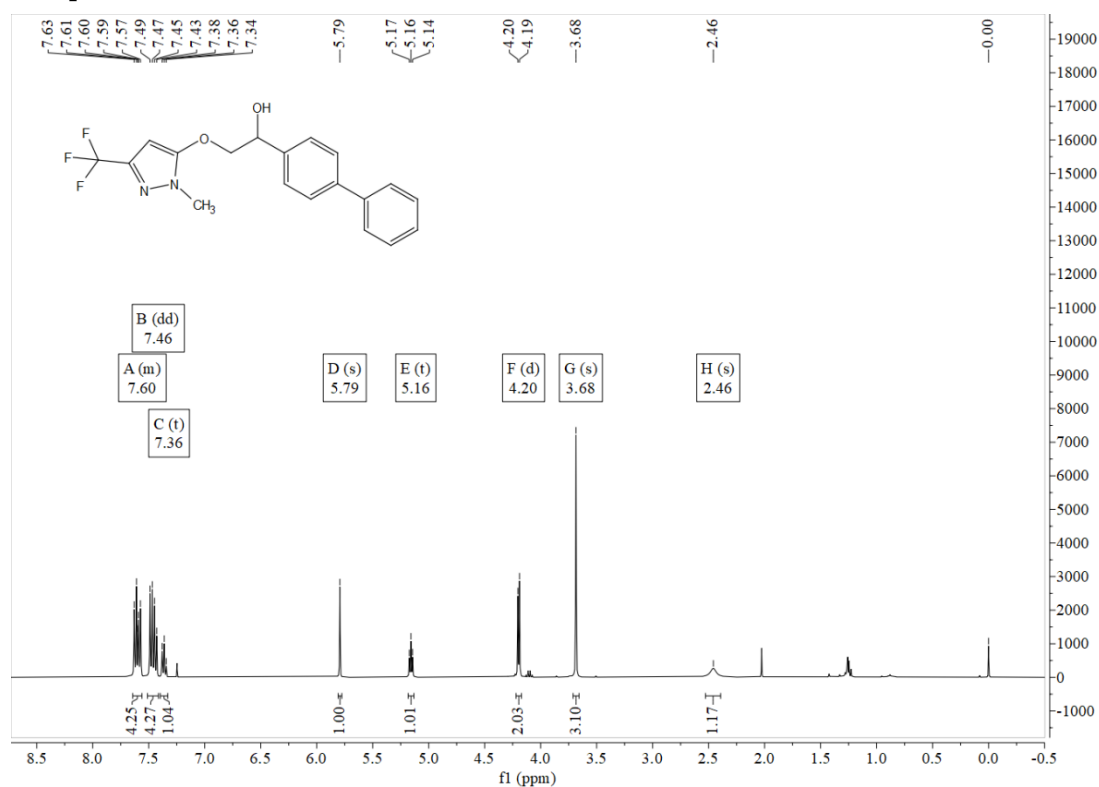


Figure 70. ¹H NMR spectrum of target compound 6x

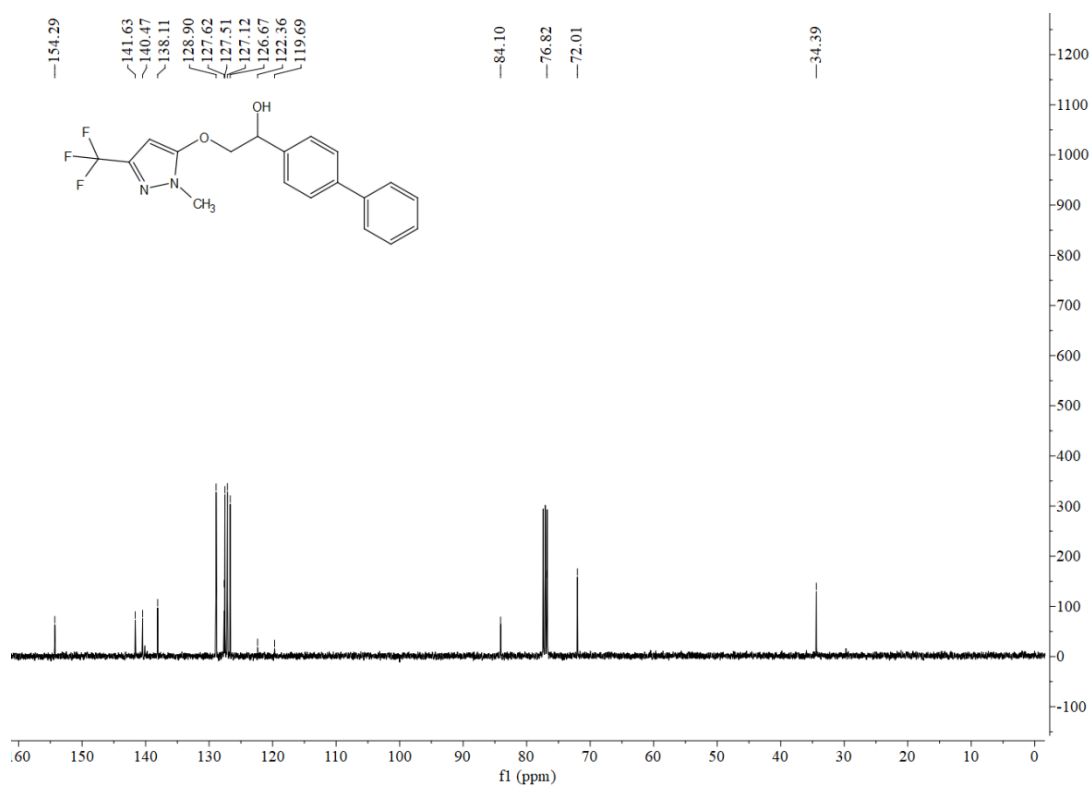


Figure 71. ¹³C NMR spectrum of target compound 6x

Spectrum from 5-4.wiff (sample 1) - Sample014, Ex...ent 1, +TOF MS (80 - 800) from 0.087 to 0.096 min

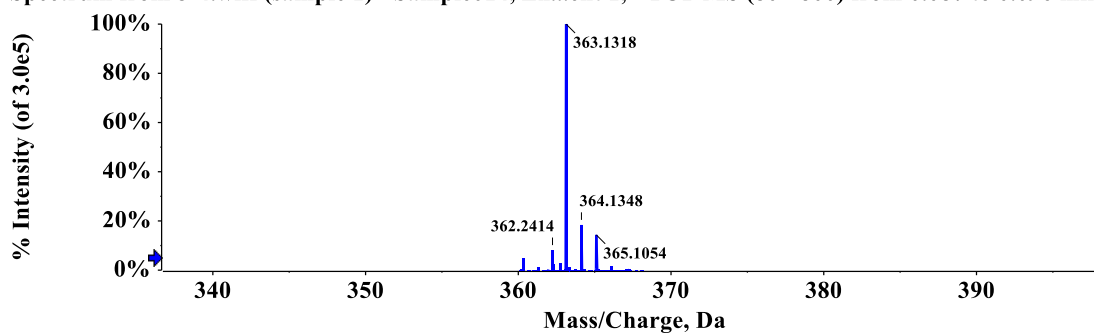


Figure 72. HRMS spectrum of target compound 6x

Compound 6y

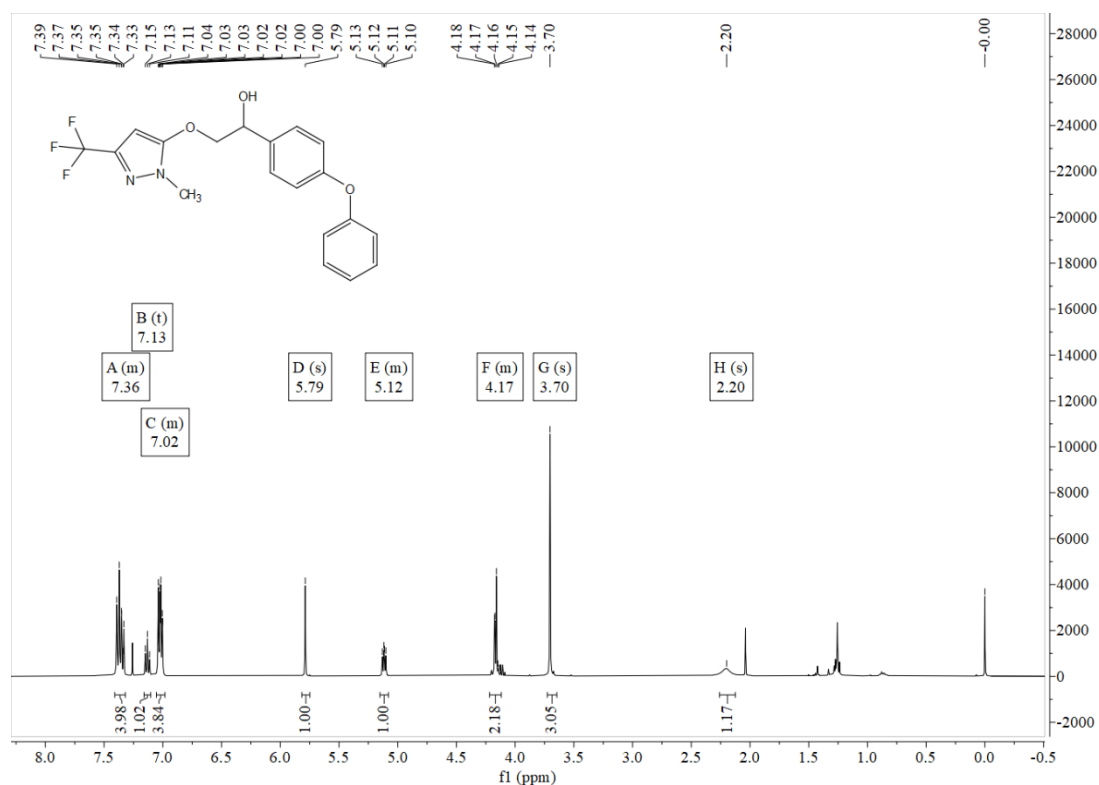


Figure 73. ¹H NMR spectrum of target compound 6y

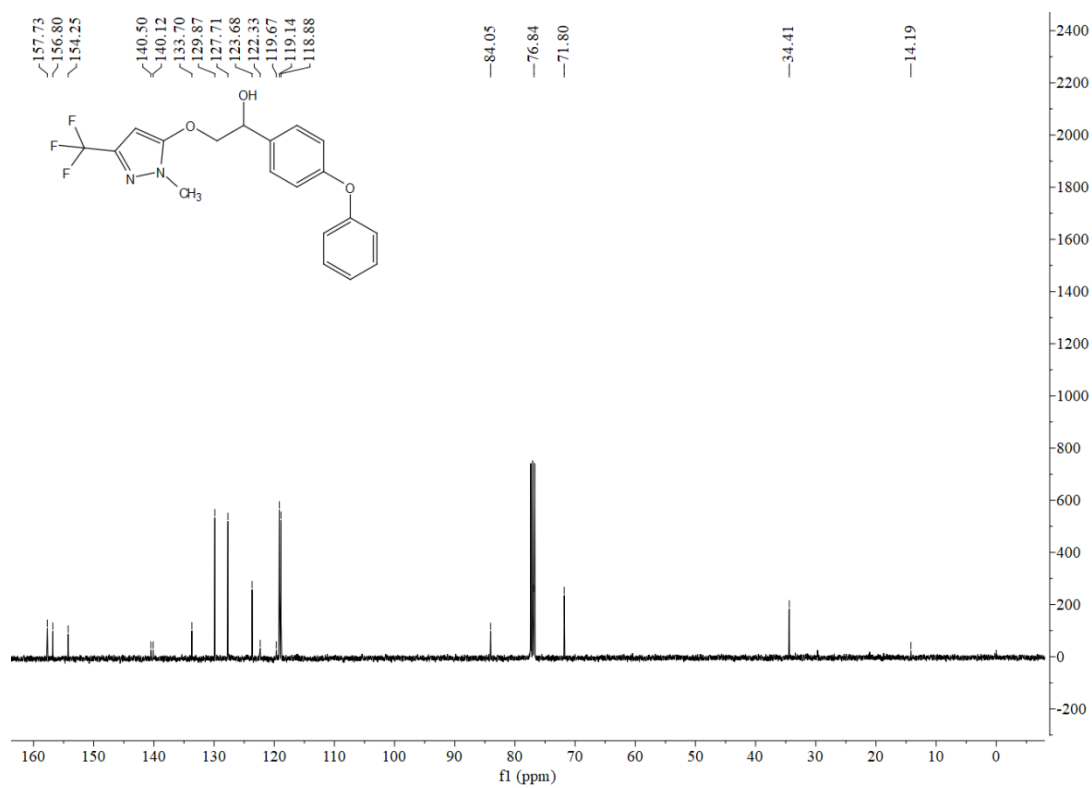


Figure 74. ¹³C NMR spectrum of target compound 6y

Spectrum from 5-7.wiff (sample 1) - Sample017, Ex...ent 1, +TOF MS (80 - 800) from 0.086 to 0.095 min

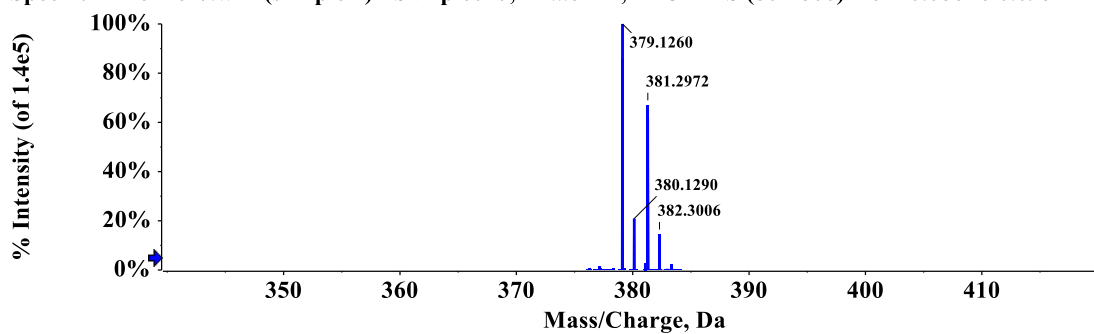


Figure 75. HRMS spectrum of target compound 6y

Compound 6z

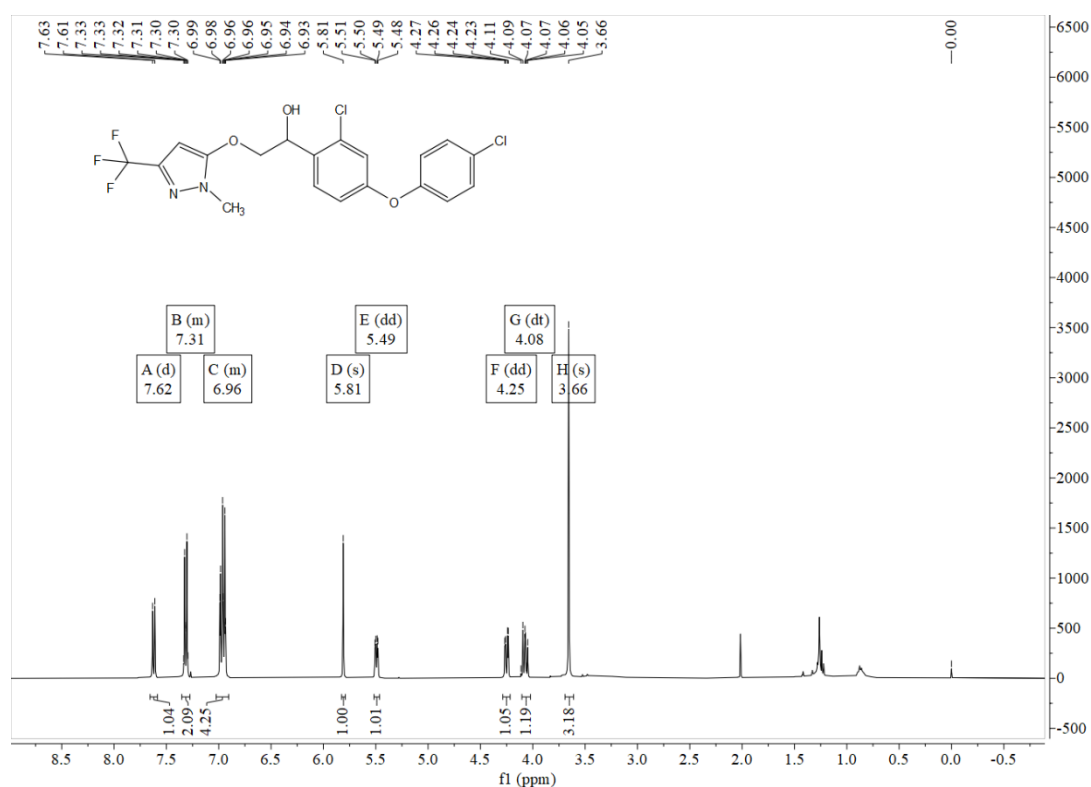


Figure 76. ¹H NMR spectrum of target compound 6z

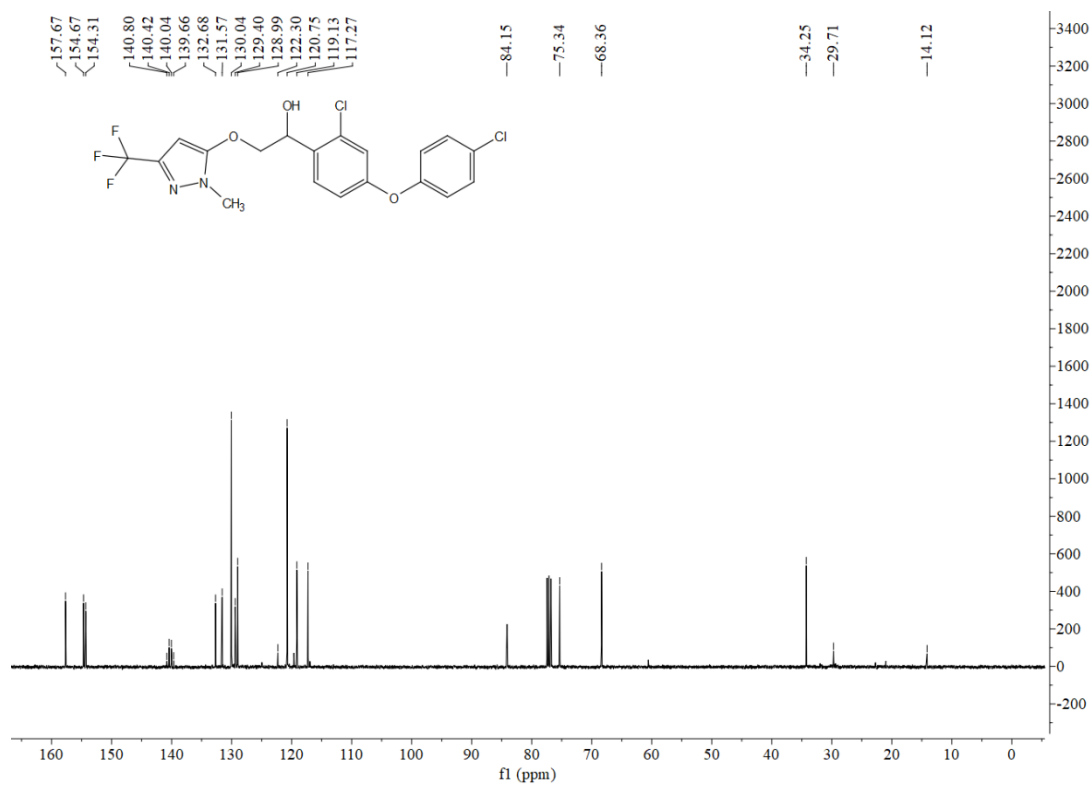


Figure 77. ¹³C NMR spectrum of target compound 6z

Spectrum from 5-8.wiff (sample 1) - Sample018, Experiment 1, +TOF MS (80 - 800) from 0.074 to 0.083 min

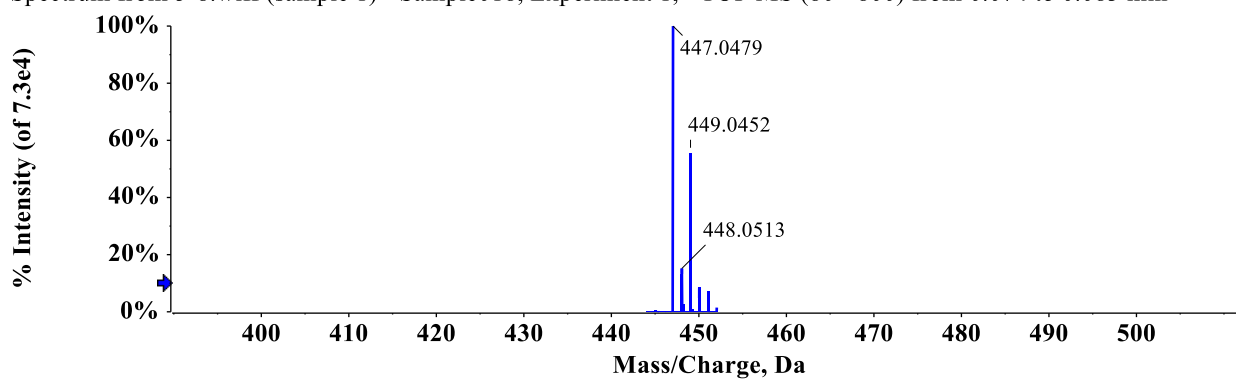


Figure 78. HRMS spectrum of target compound 6z