

Supplementary information

Carbonylation of Polyfluorinated Alkylbenzenes and Benzocycloalkenes at the Benzyl C-F and C-Cl Bonds under the Action of CO/SbF₅

Yaroslav V. Zonov ^{1,2,*}, Siqu Wang ³, Vladislav V. Komarov ¹, Victor M. Karpov ¹, Dmitriy A. Parkhomenko ¹ and Tatyana V. Mezhenkova ¹

¹ N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS, Lavrentiev Ave. 9, Novosibirsk 630090, Russia

² Department of Natural Sciences, Novosibirsk State University, Pirogov Str. 1, Novosibirsk 630090, Russia

³ Daqing Petrochemical Research Center, PetroChina Company Limited, Daqing 163714, China

* Correspondence: yzonov@nioch.nsc.ru

¹H and ¹⁹F NMR spectra of products

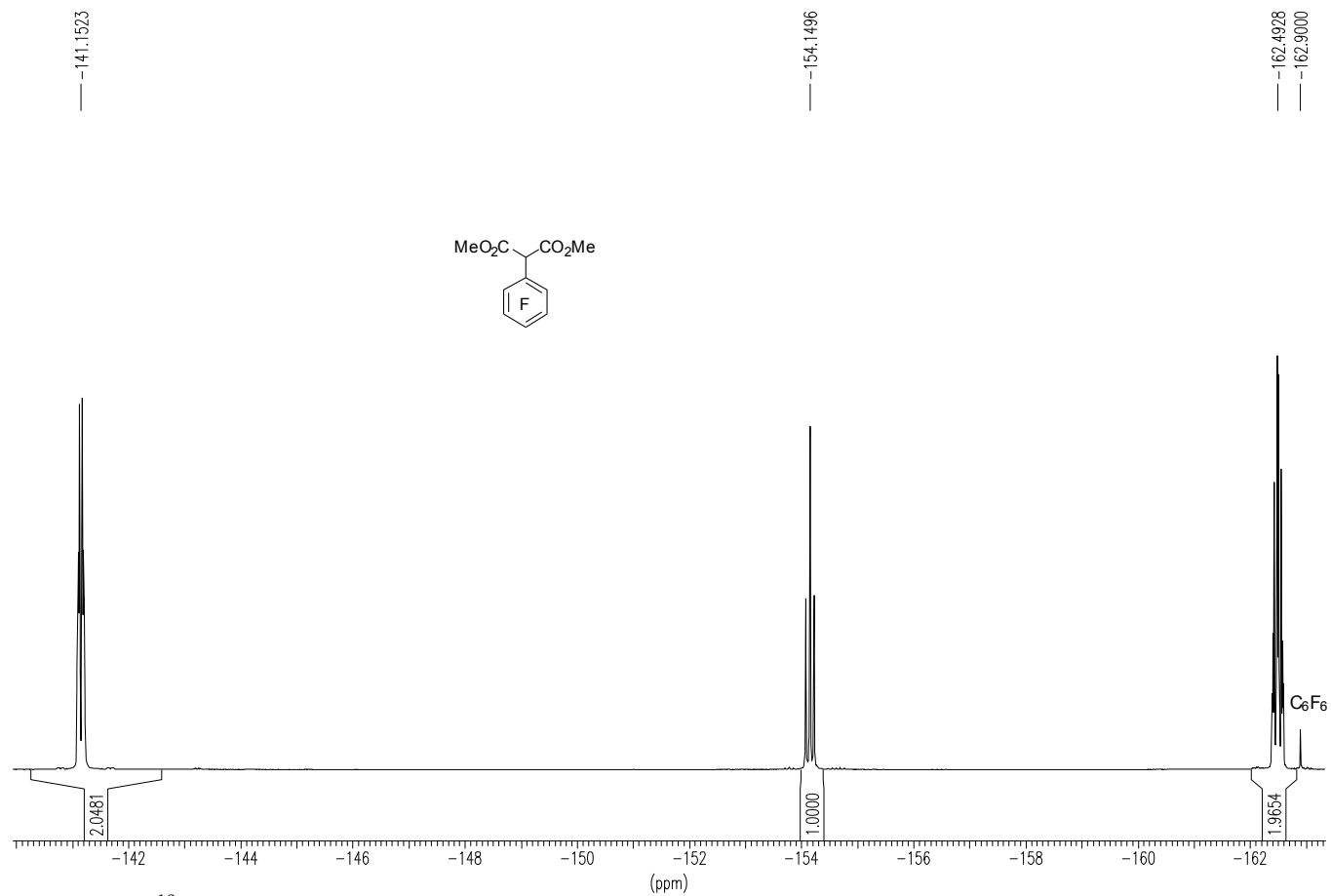


Figure S1. ¹⁹F NMR spectrum of **3'a** (CDCl₃).

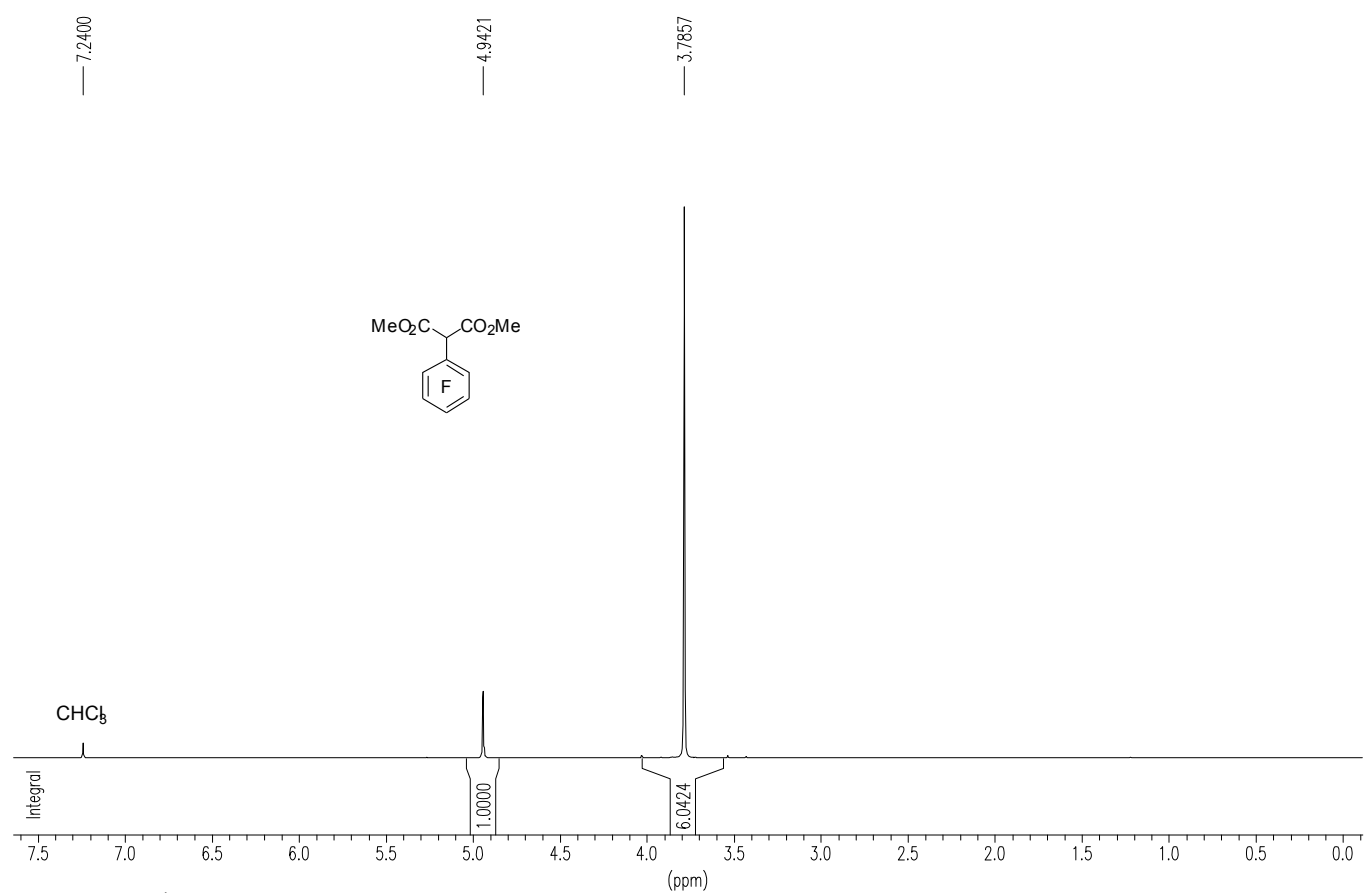


Figure S2. ¹H NMR spectrum of **3'a** (CDCl₃).

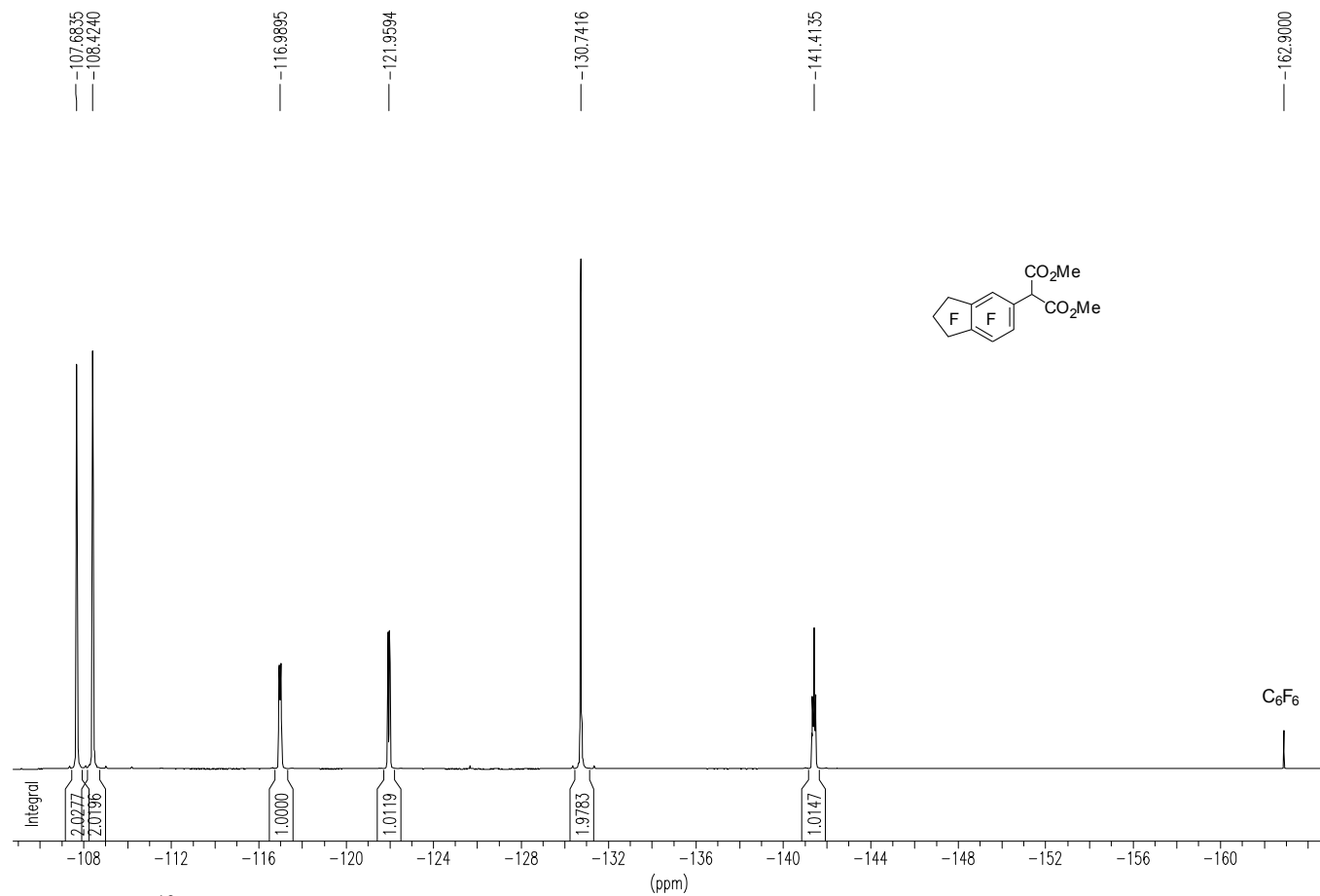


Figure S3. ¹⁹F NMR spectrum of **3'b** (CDCl₃).

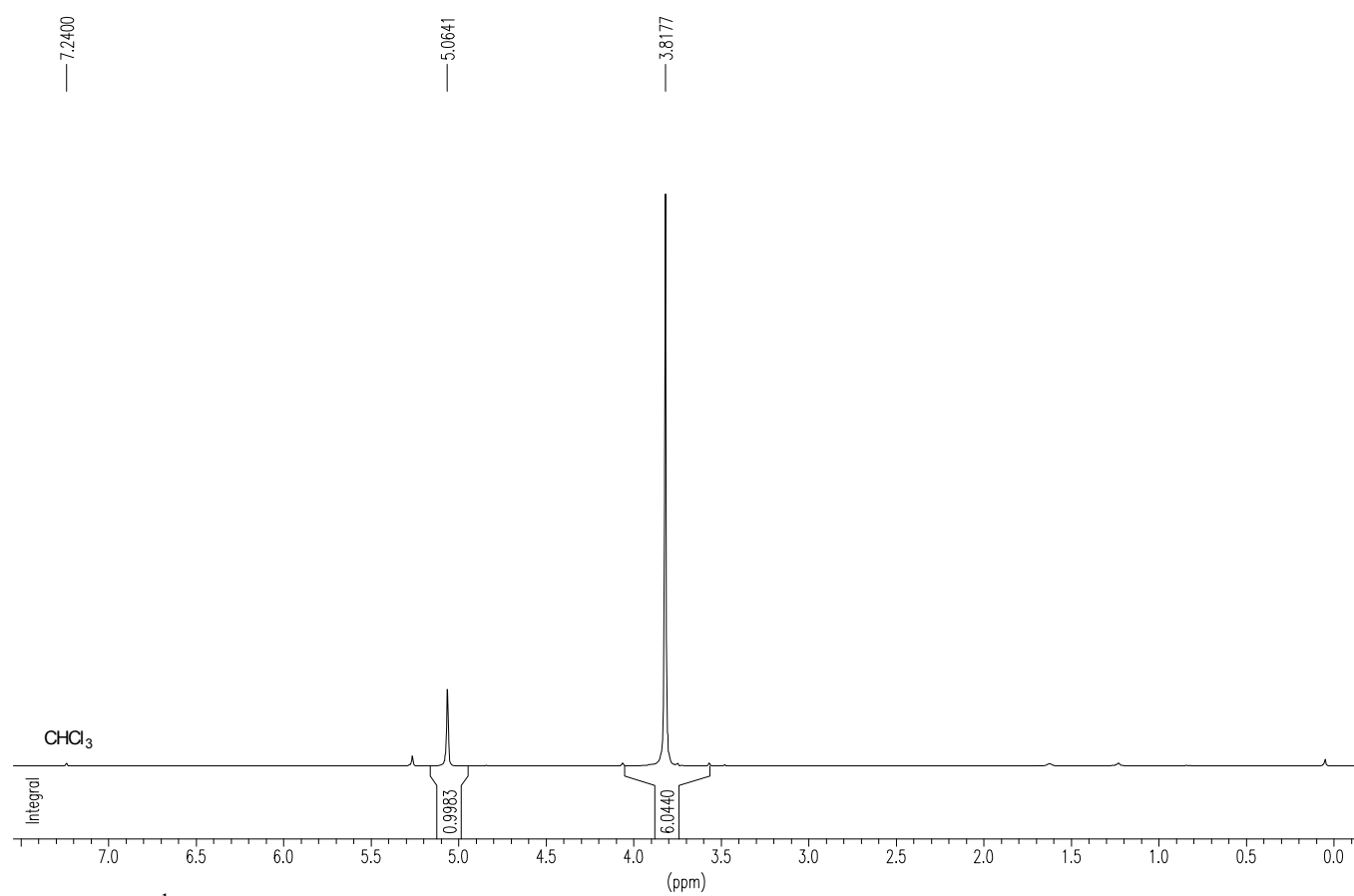


Figure S4. ¹H NMR spectrum of **3'b** (CDCl₃).

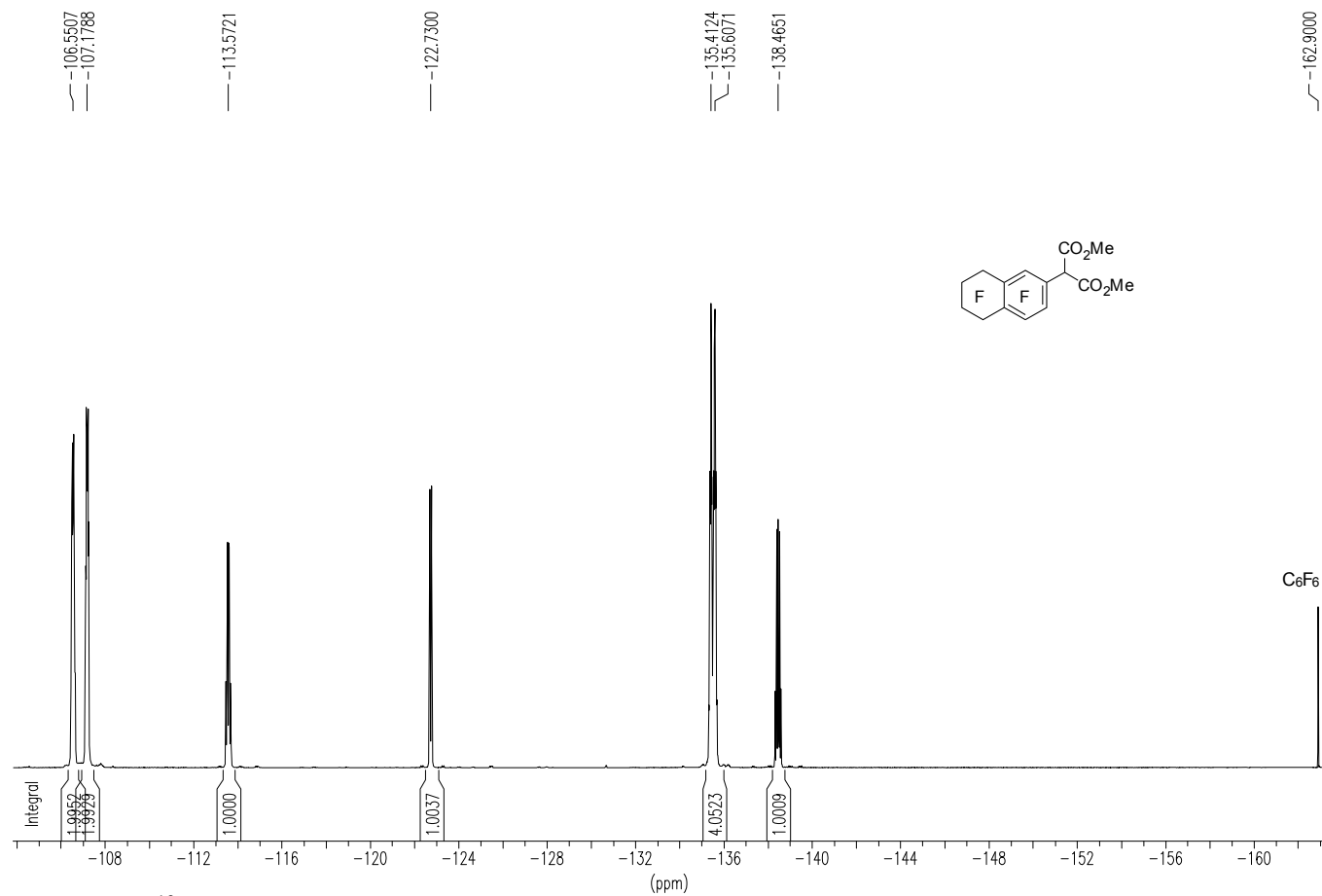


Figure S5. ¹⁹F NMR spectrum of **3'c** (CDCl₃).

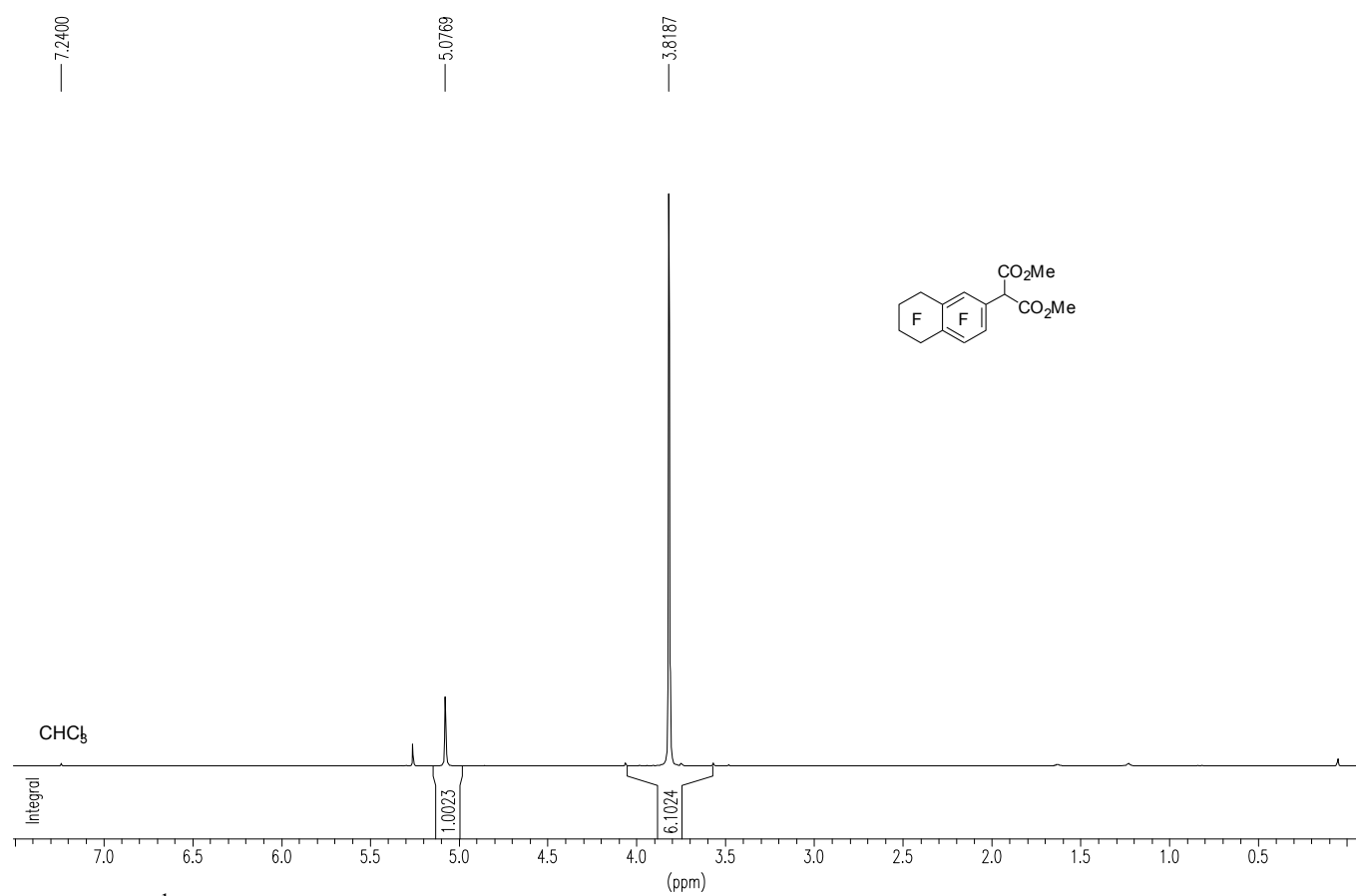


Figure S6. ¹H NMR spectrum of **3'c** (CDCl₃).

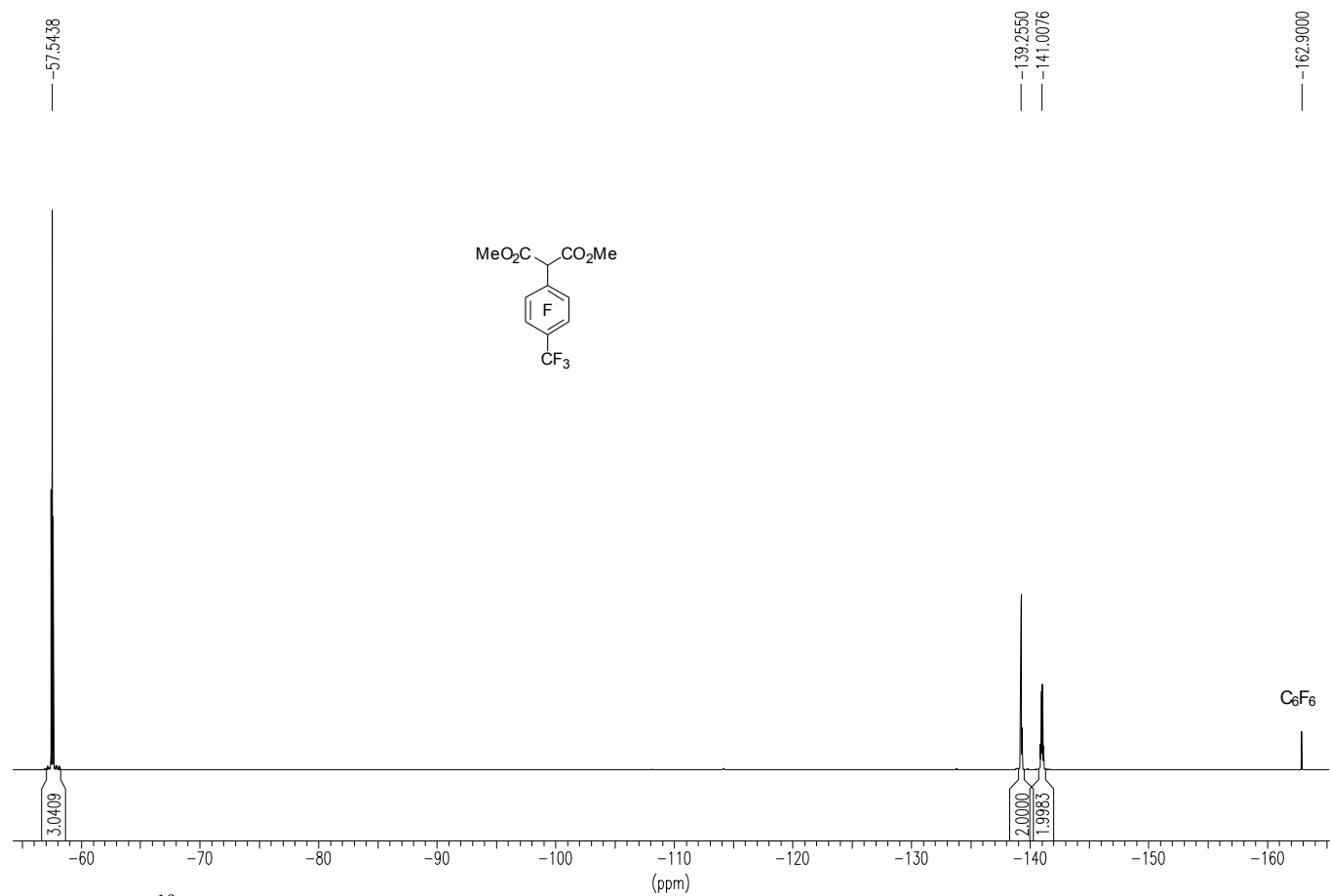


Figure S7. ¹⁹F NMR spectrum of **3'd** (CDCl₃).

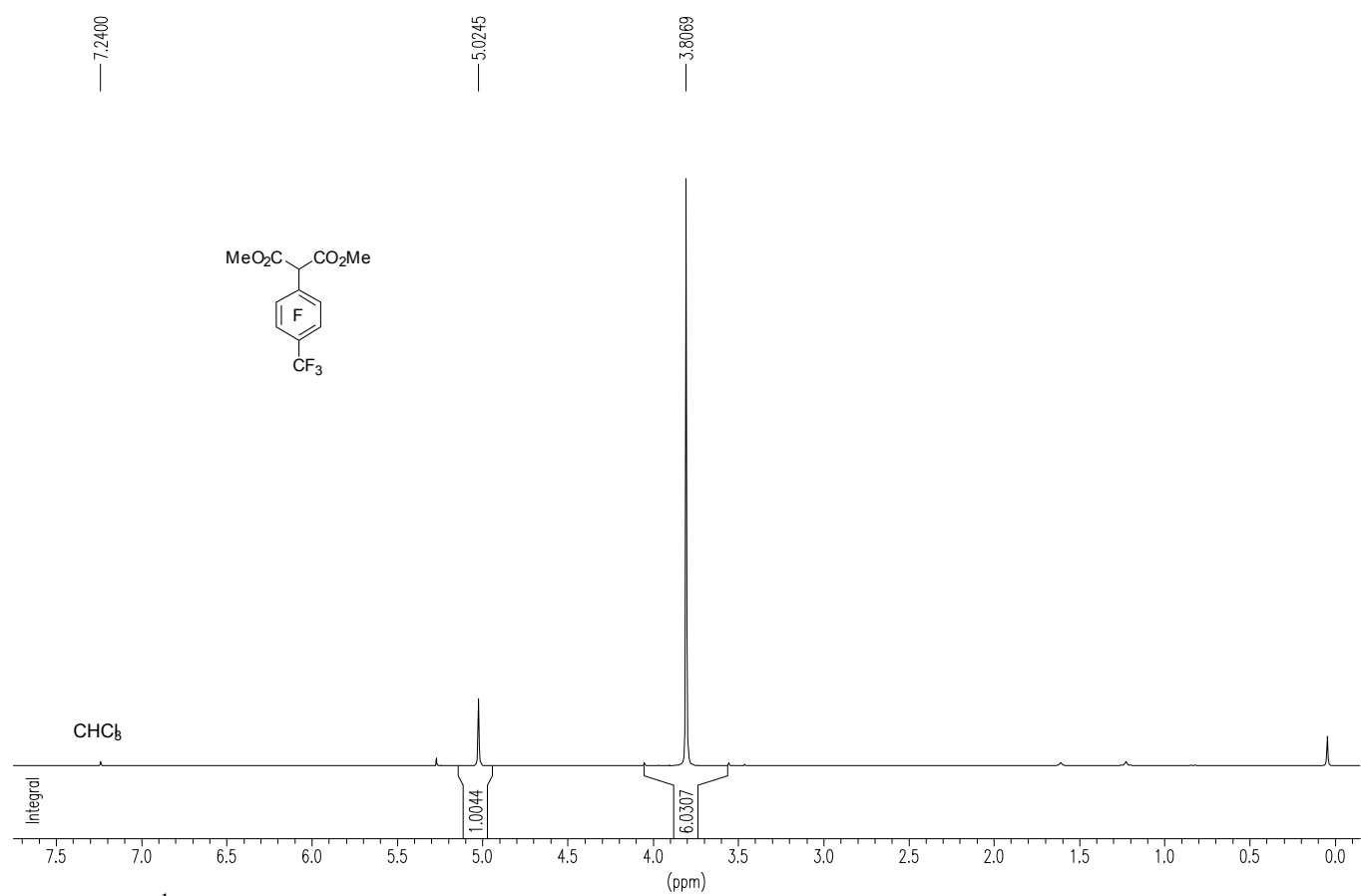


Figure S8. ¹H NMR spectrum of **3'd** (CDCl₃).

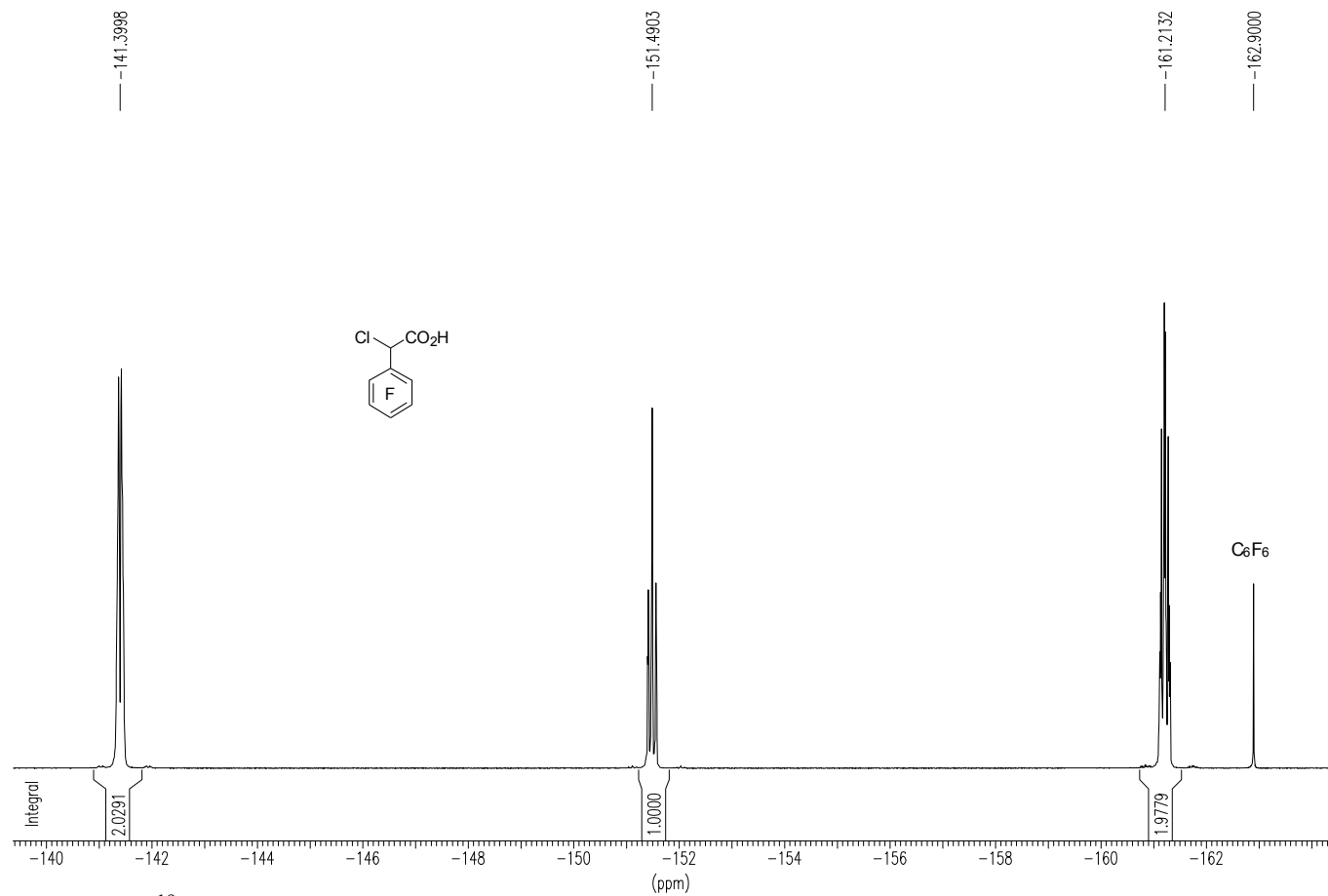


Figure S9. ¹⁹F NMR spectrum of **6a** (CDCl₃).

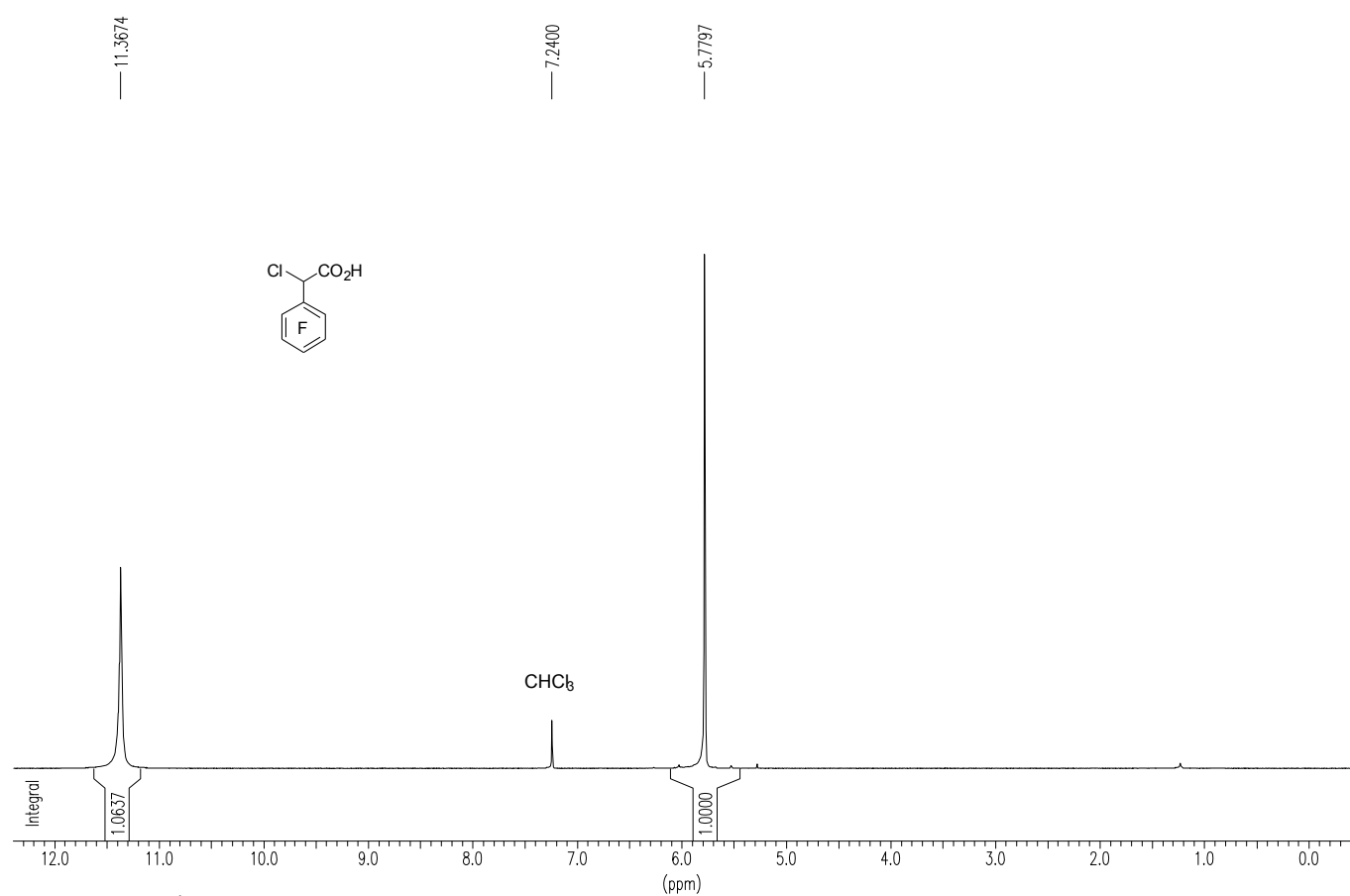


Figure S10. ¹H NMR spectrum of **6a** (CDCl₃).

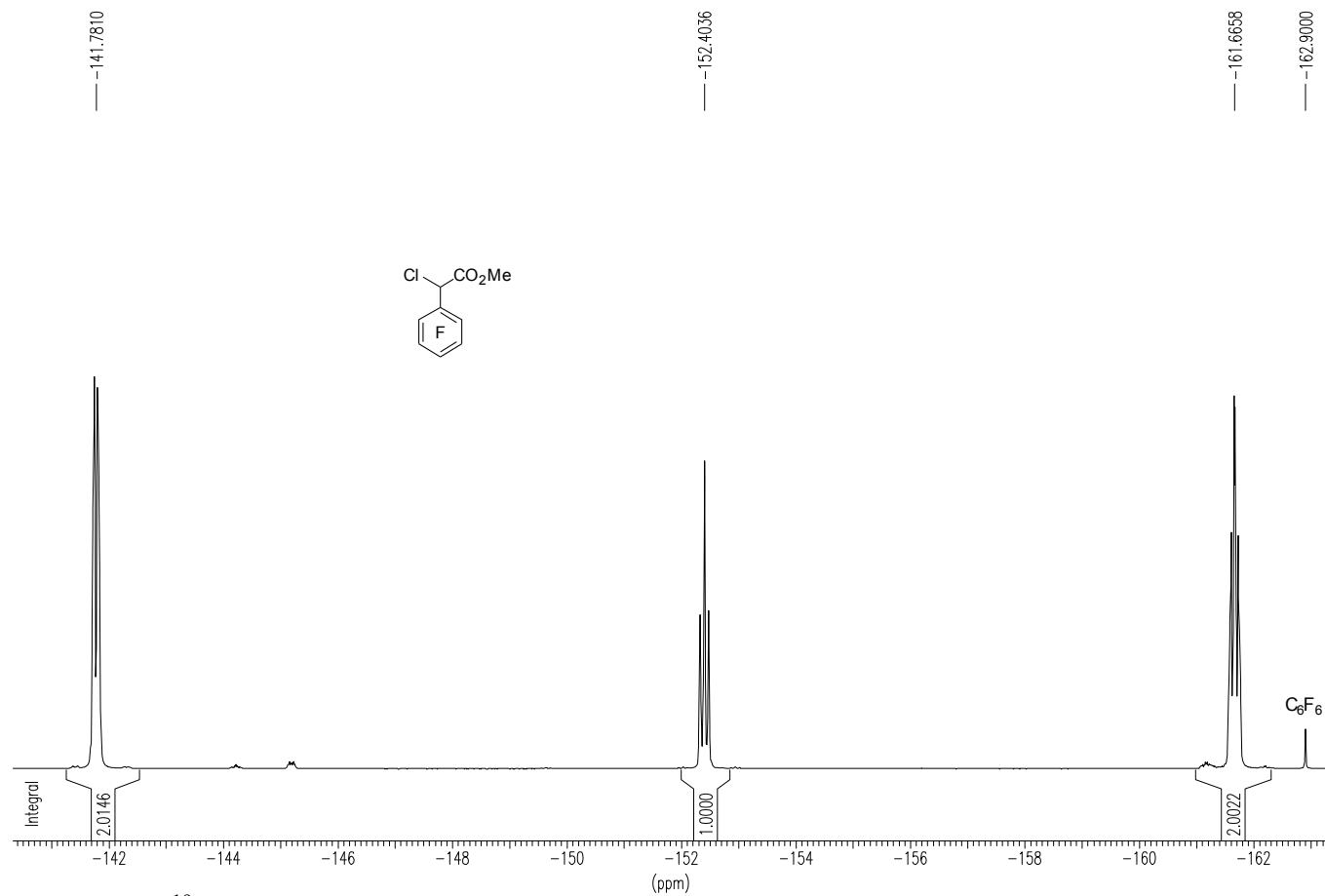


Figure S11. ¹⁹F NMR spectrum of **6'a** (CDCl₃).

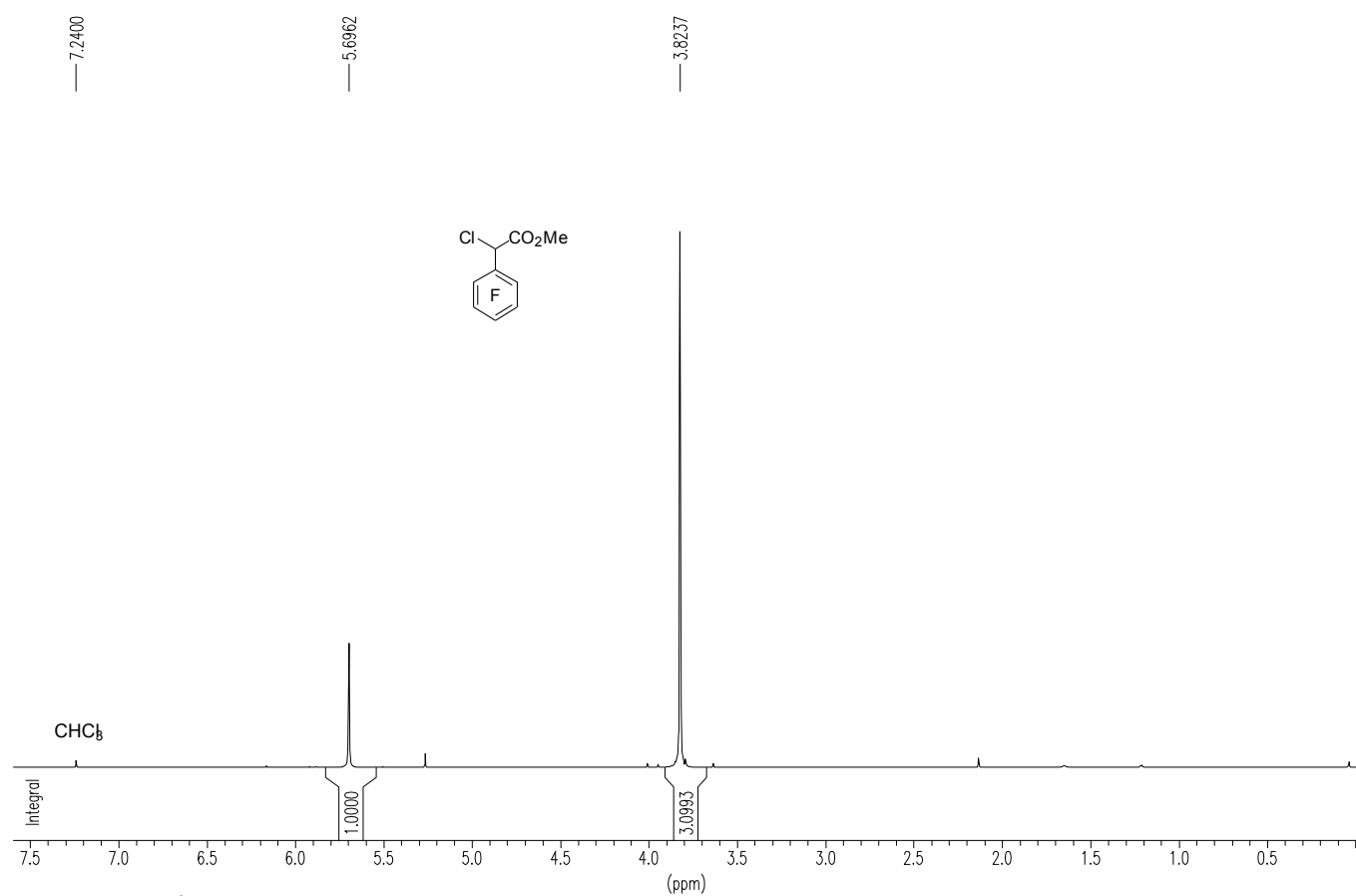


Figure S12. ¹H NMR spectrum of **6'a** (CDCl₃).

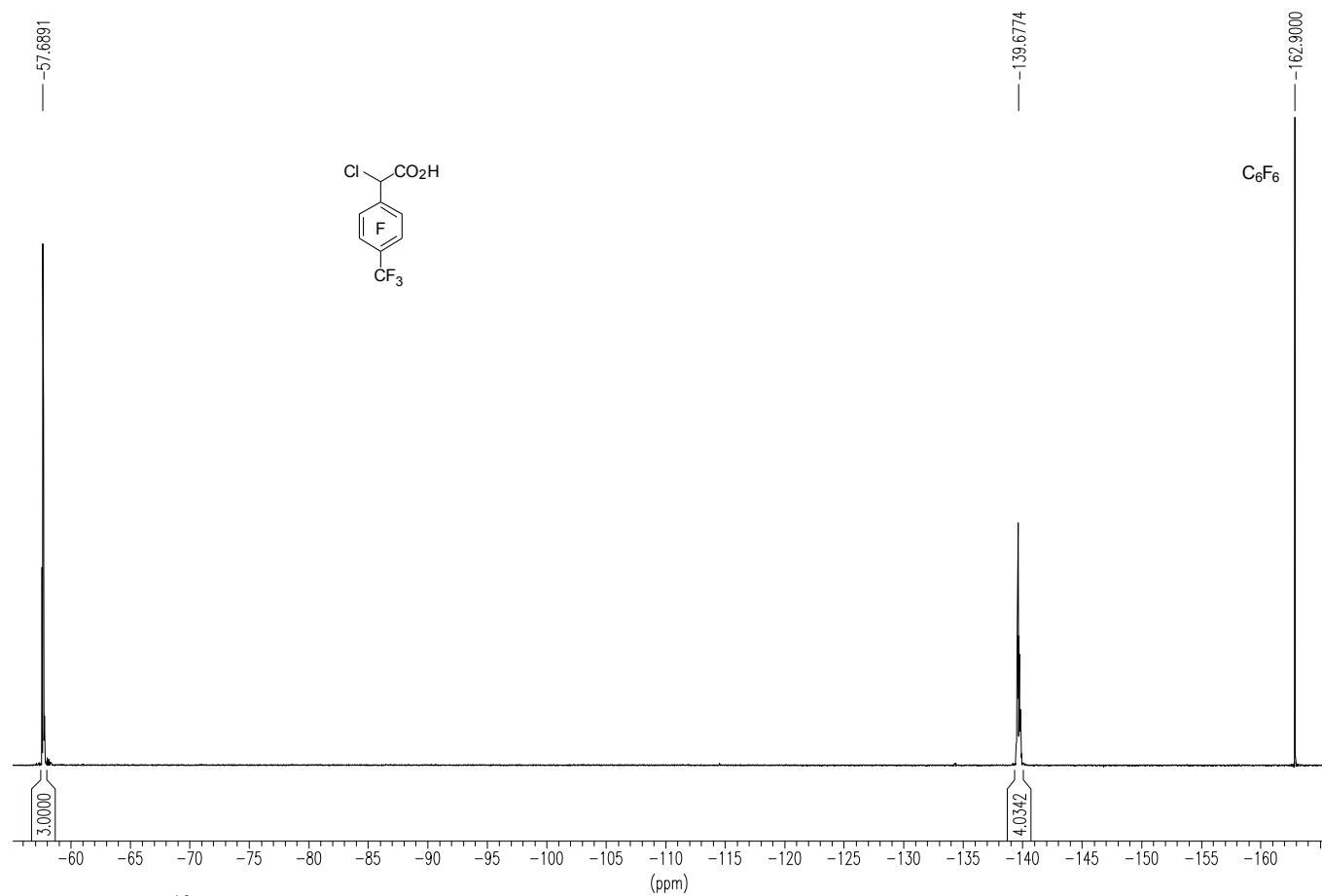


Figure S13. ^{19}F NMR spectrum of **6d** (CDCl_3).

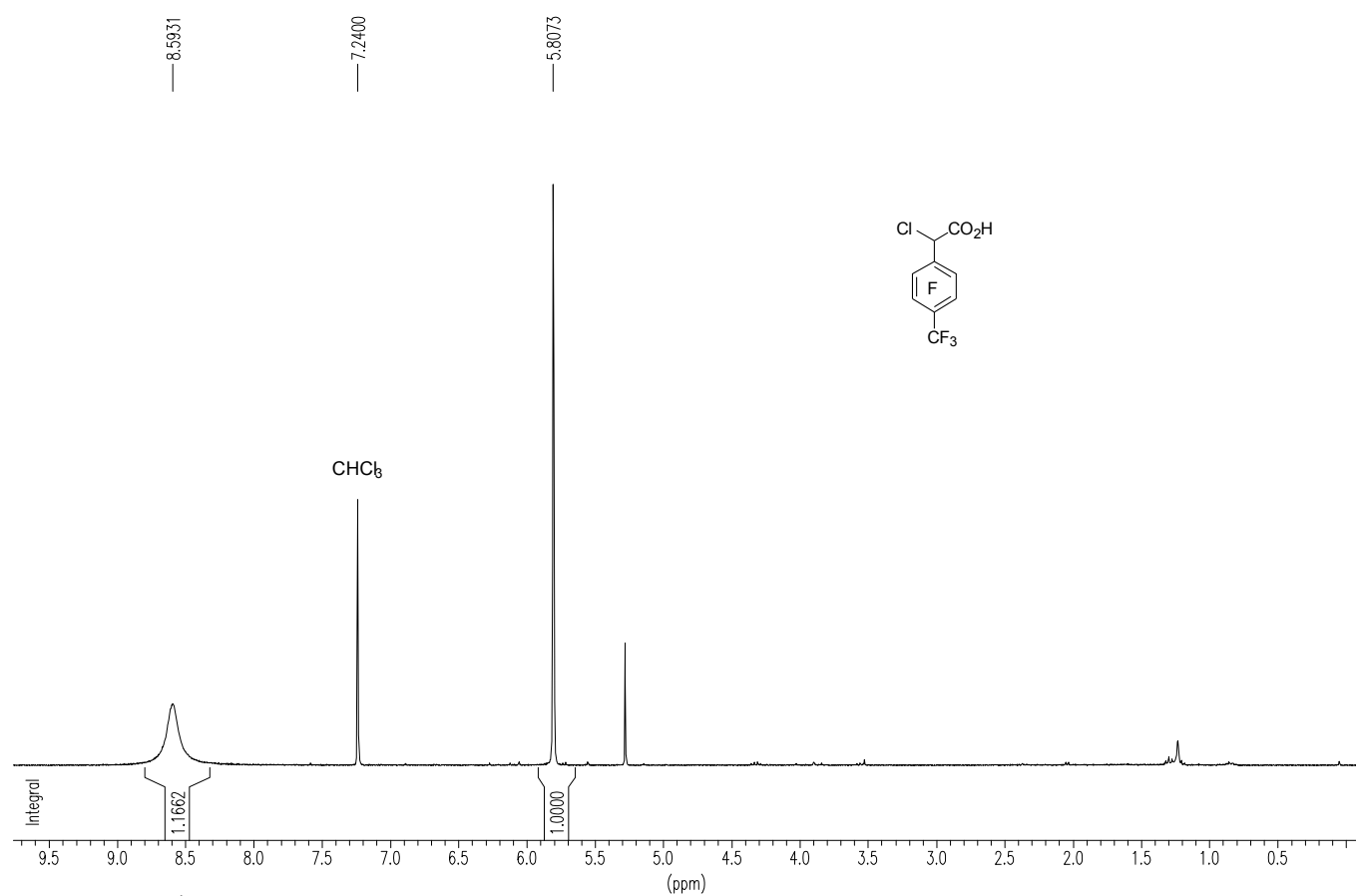


Figure S14. ^1H NMR spectrum of **6d** (CDCl_3).

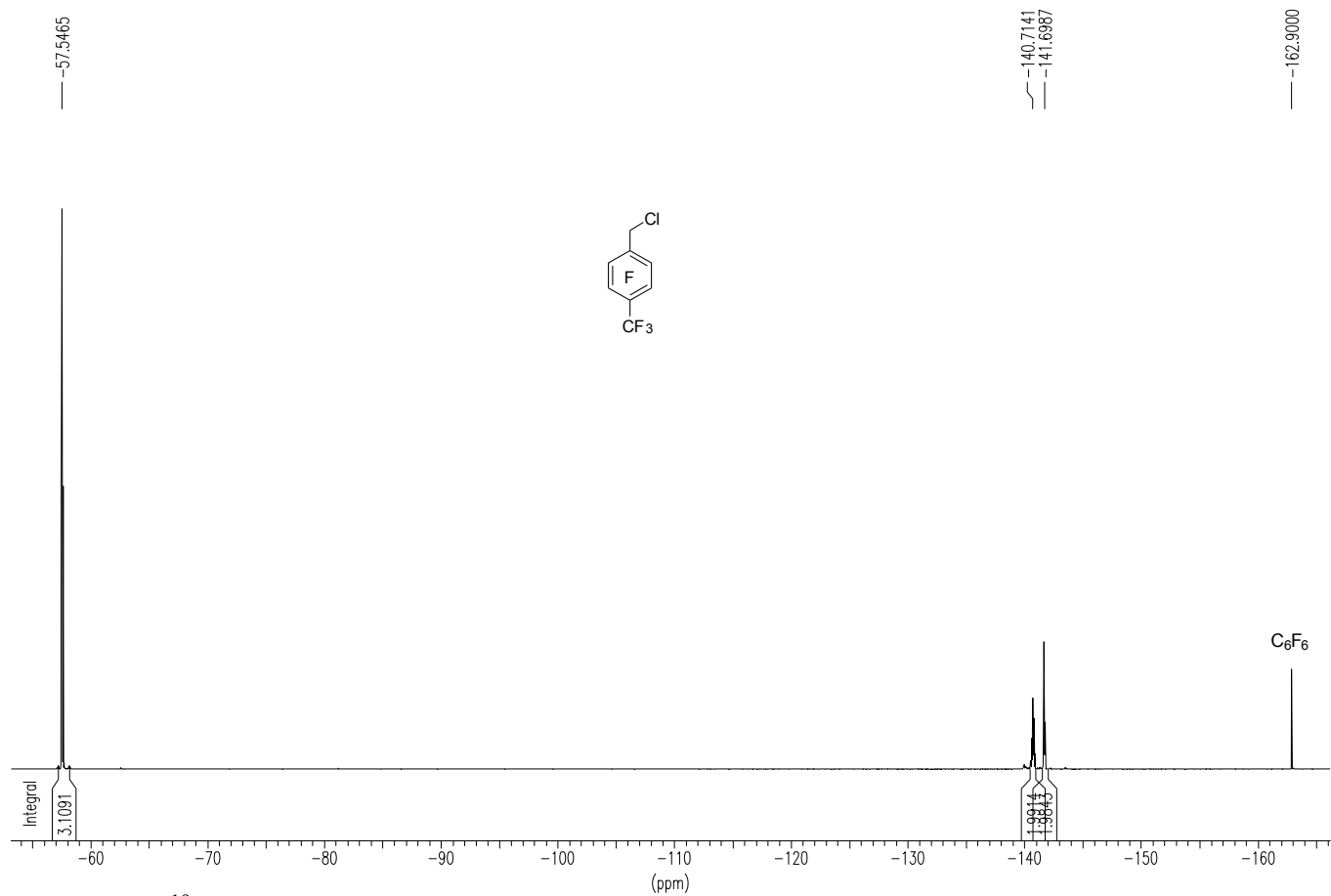


Figure S15. ¹⁹F NMR spectrum of **8d** (CDCl₃).

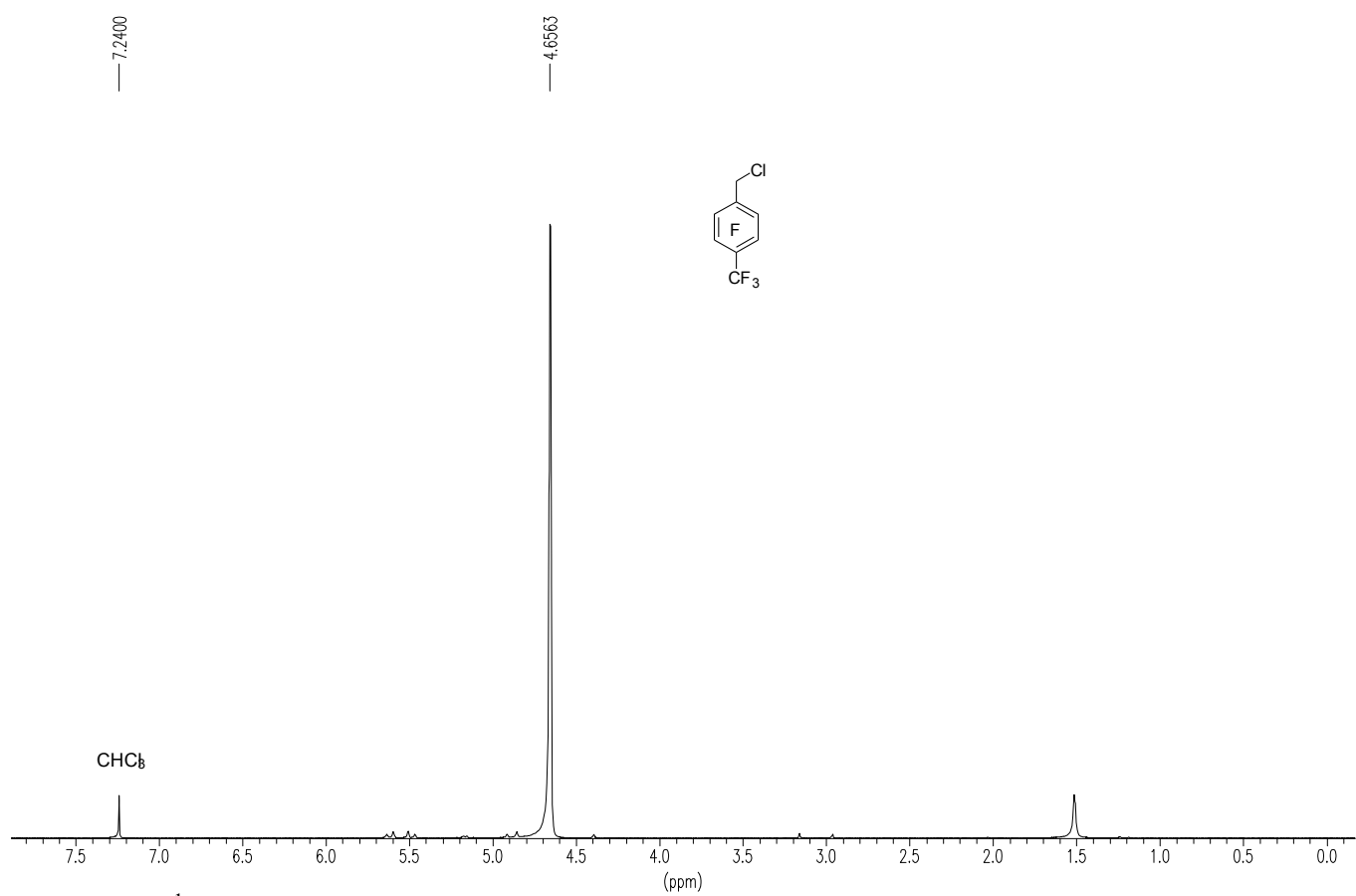


Figure S16. ¹H NMR spectrum of **8d** (CDCl₃).

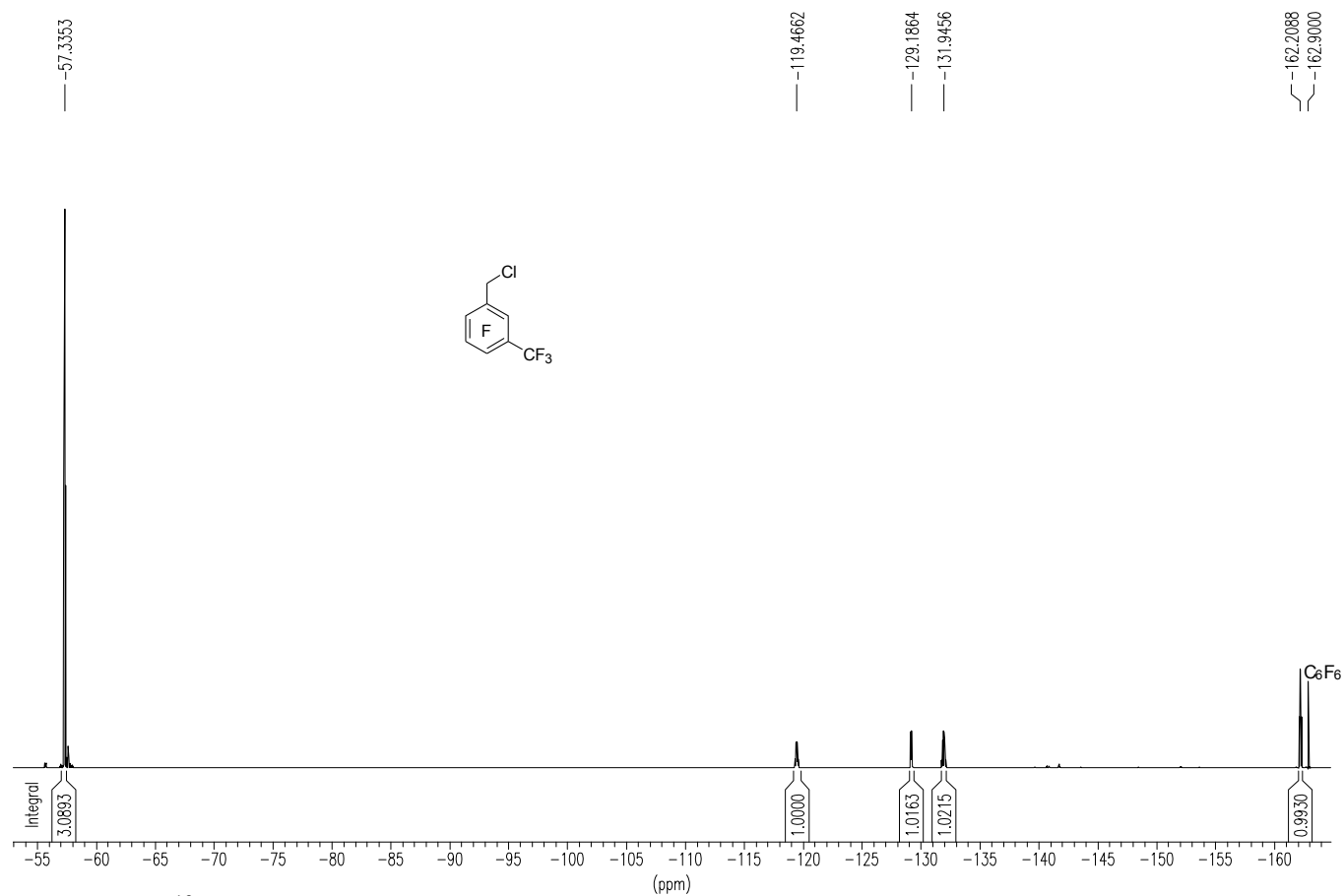


Figure S17. ^{19}F NMR spectrum of **8e** (CDCl_3).

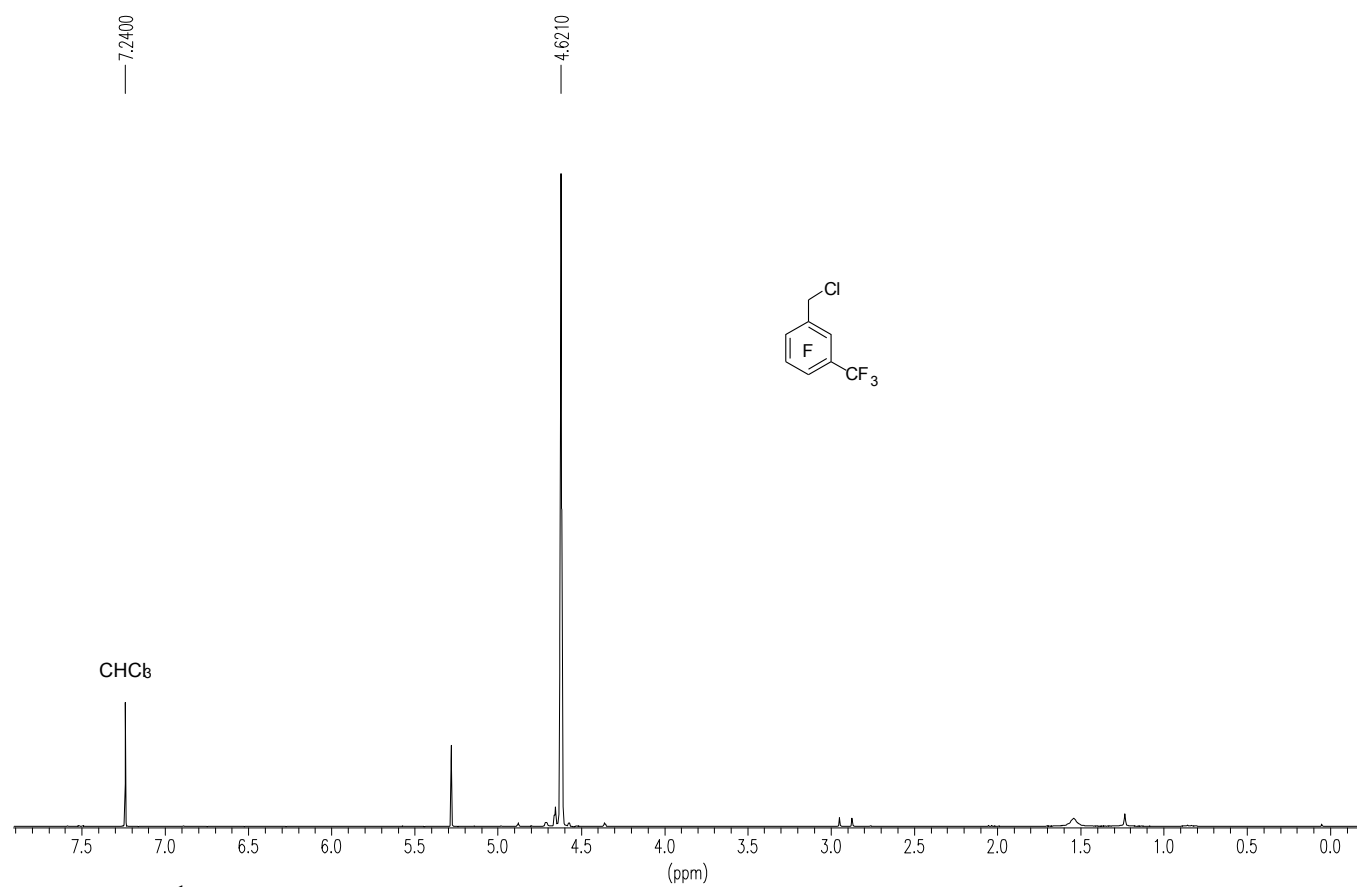


Figure S18. ^1H NMR spectrum of **8e** (CDCl_3).

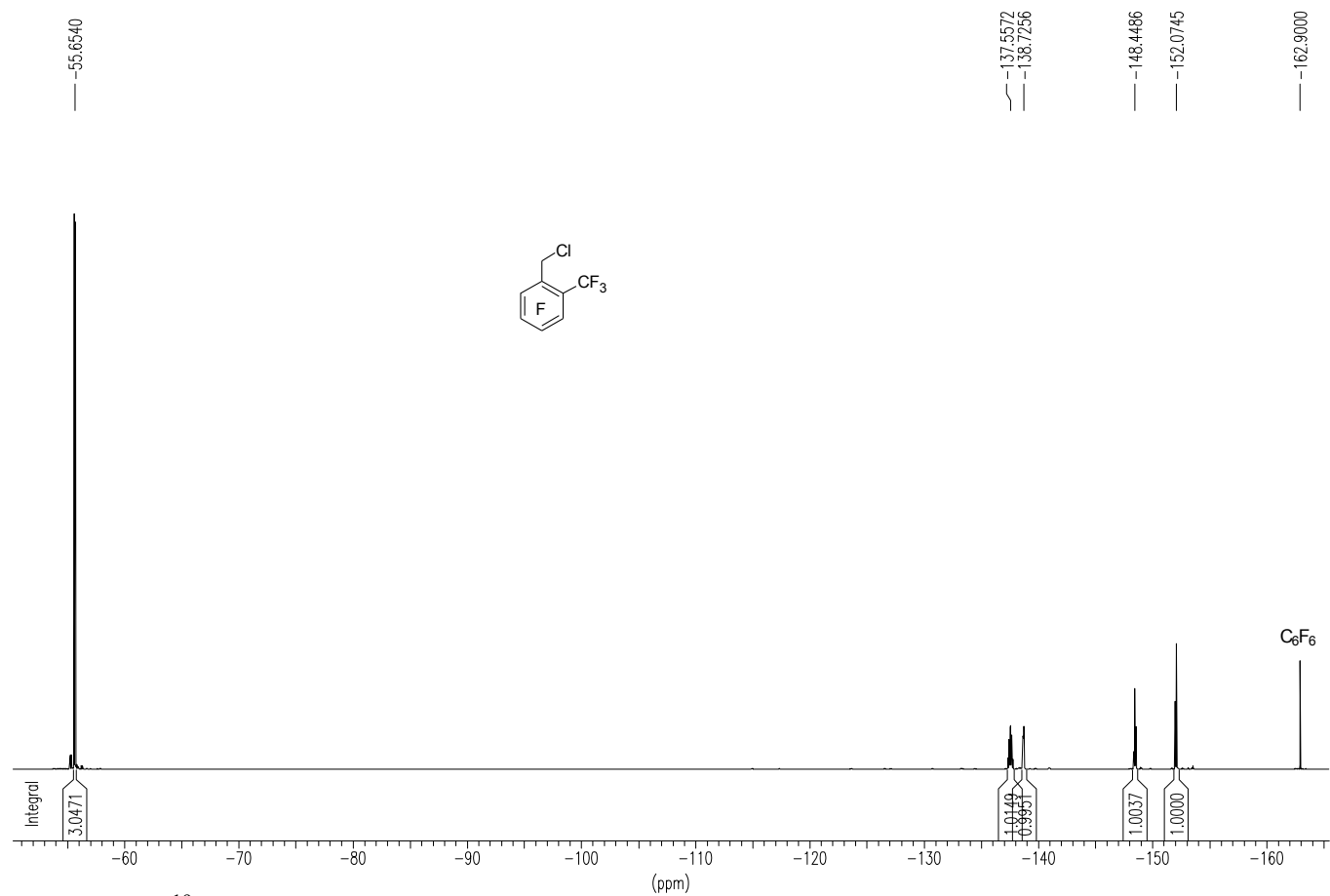


Figure S19. ¹⁹F NMR spectrum of **8f** (CDCl₃).

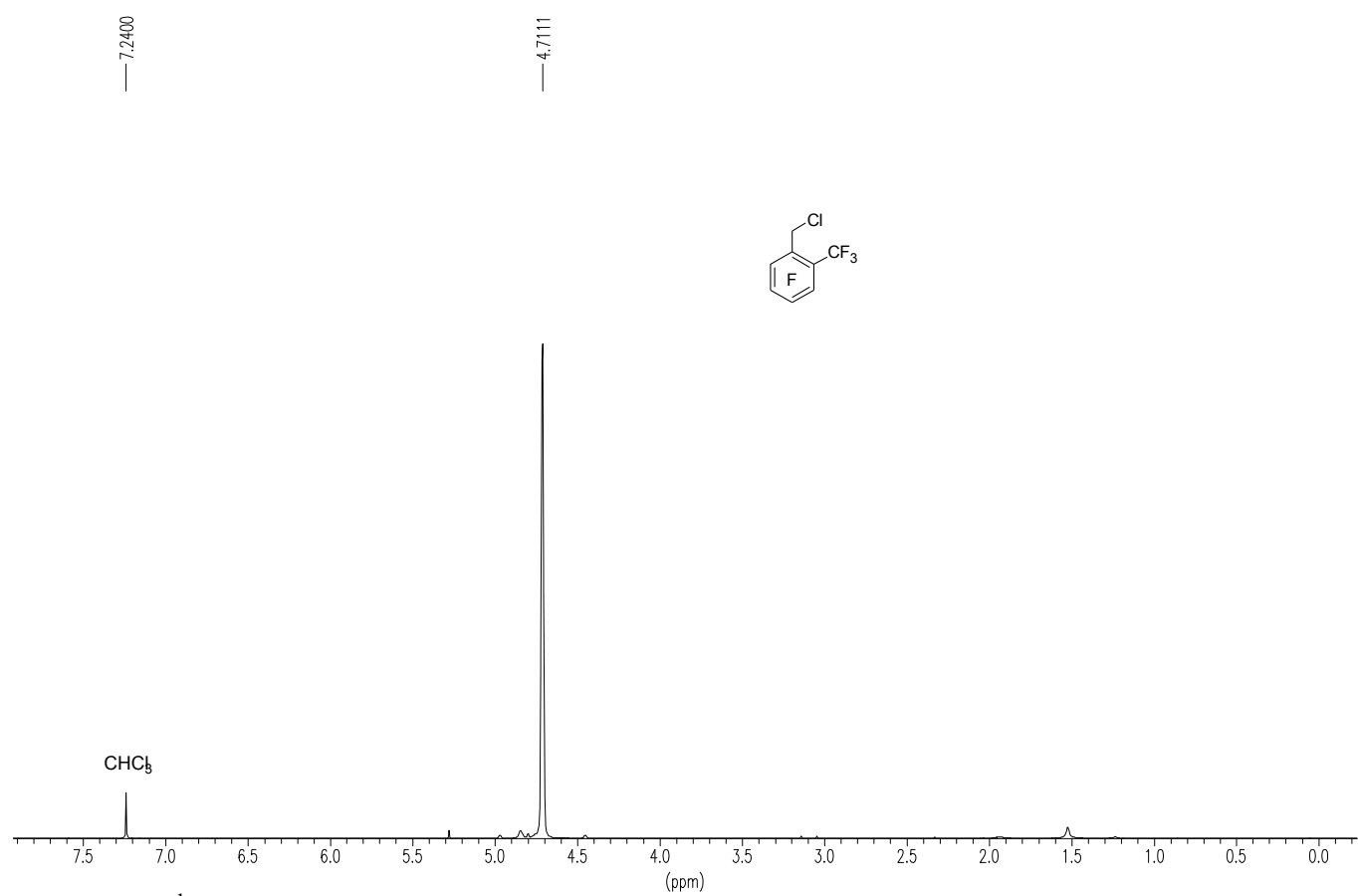


Figure S20. ¹H NMR spectrum of **8f** (CDCl₃).

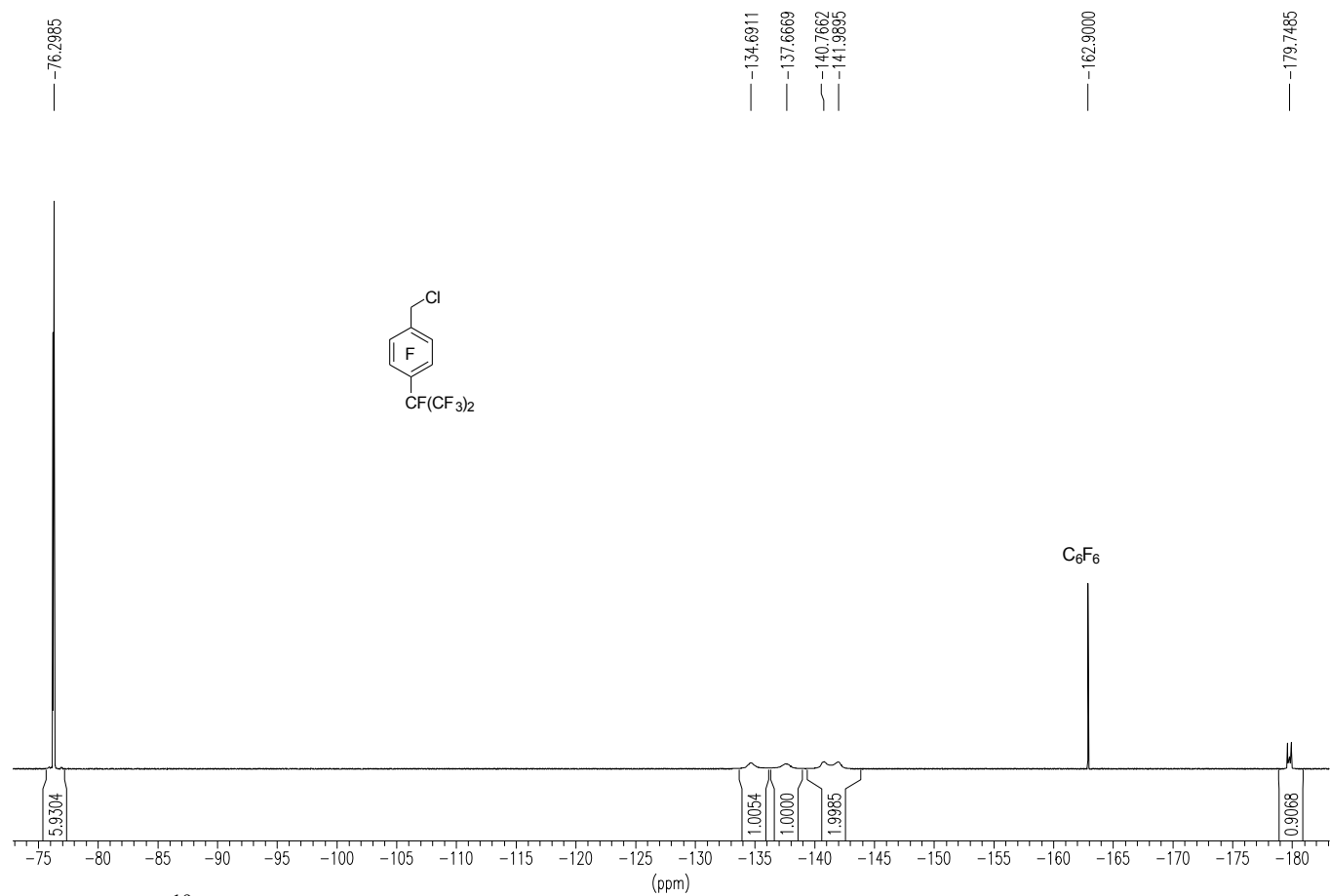


Figure S21. ¹⁹F NMR spectrum of **8g** (CDCl₃).

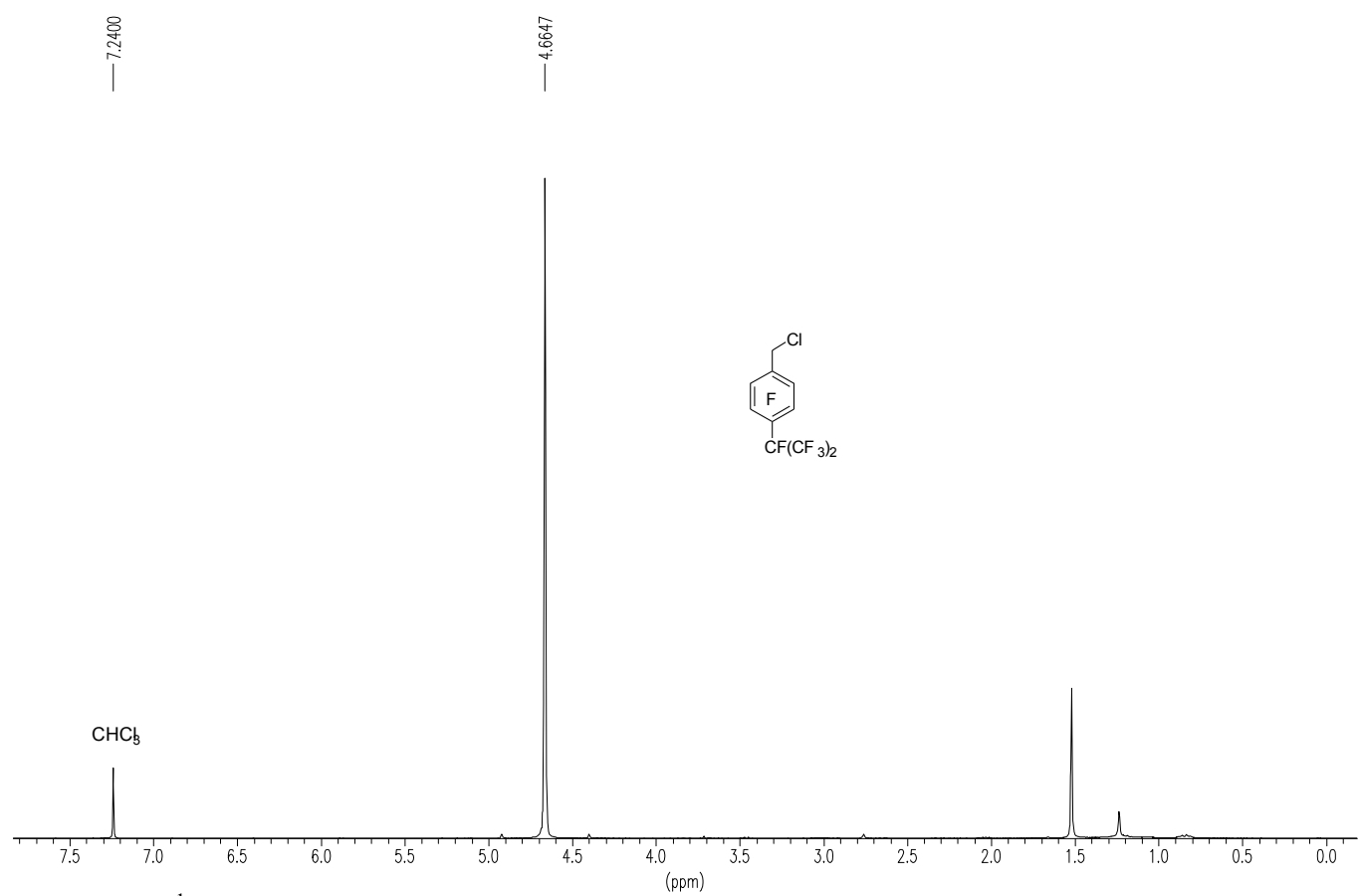


Figure S22. ¹H NMR spectrum of **8g** (CDCl₃).

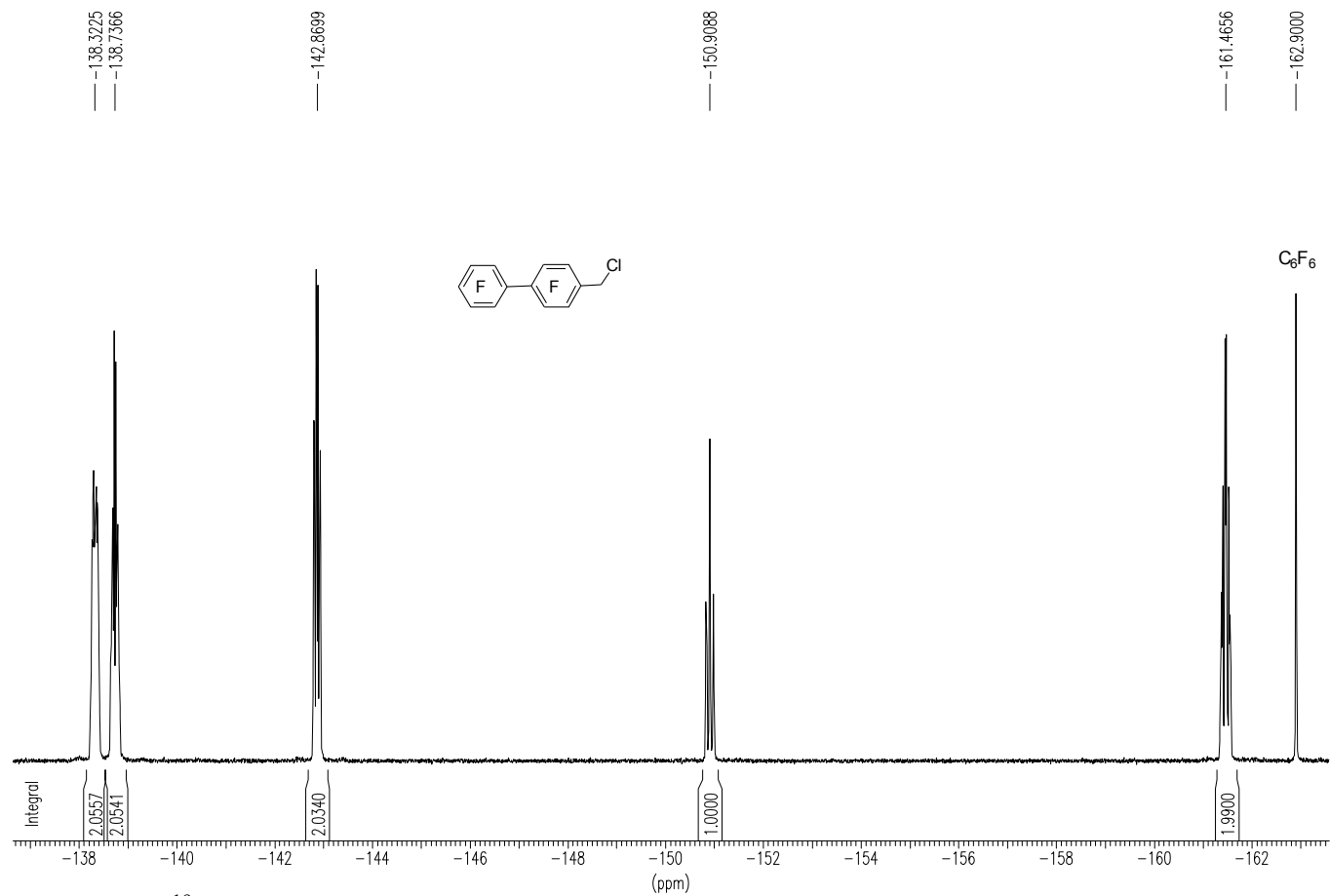


Figure S23. ¹⁹F NMR spectrum of **8h** (CDCl₃).

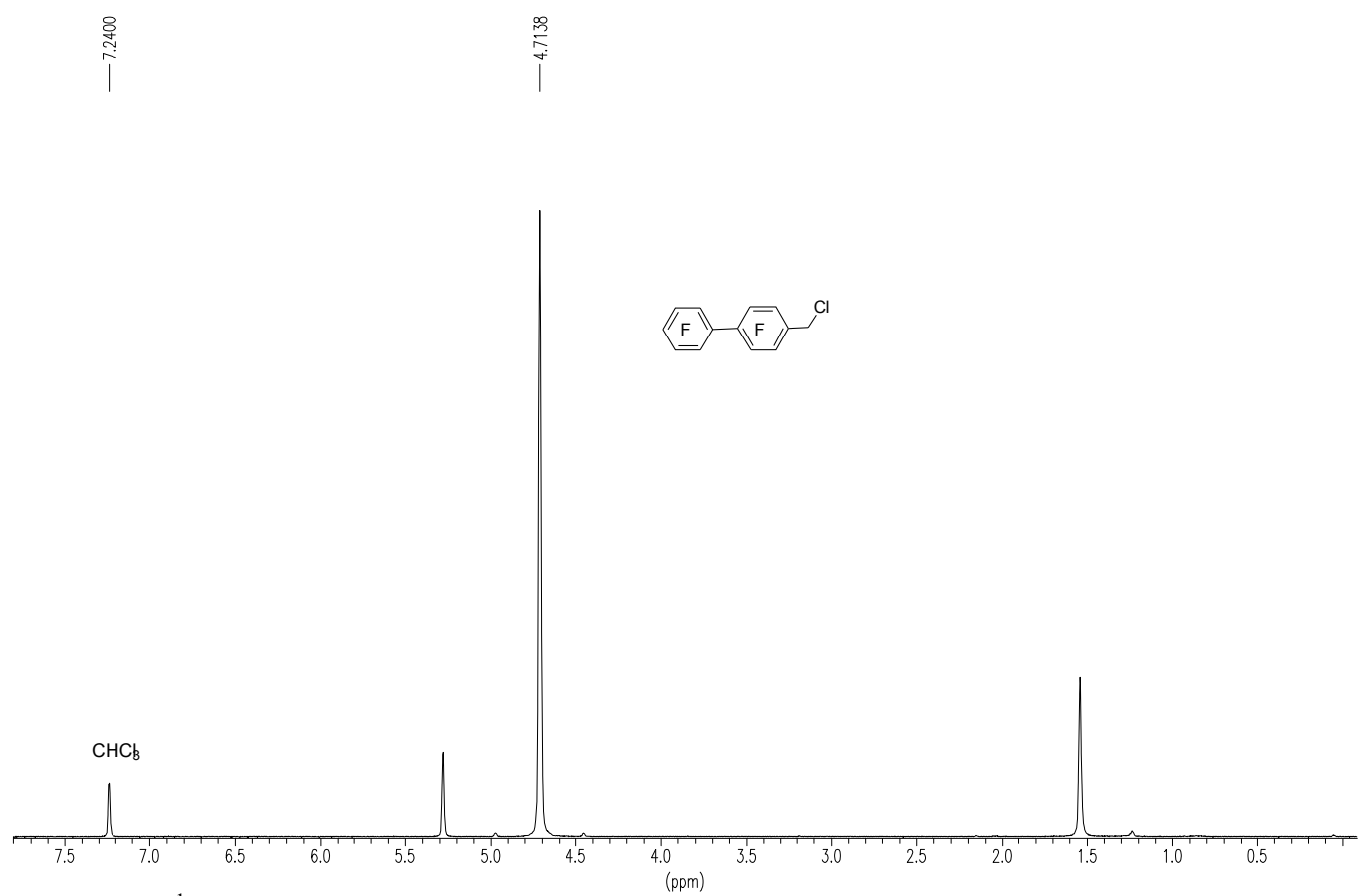


Figure S24. ¹H NMR spectrum of **8h** (CDCl₃).

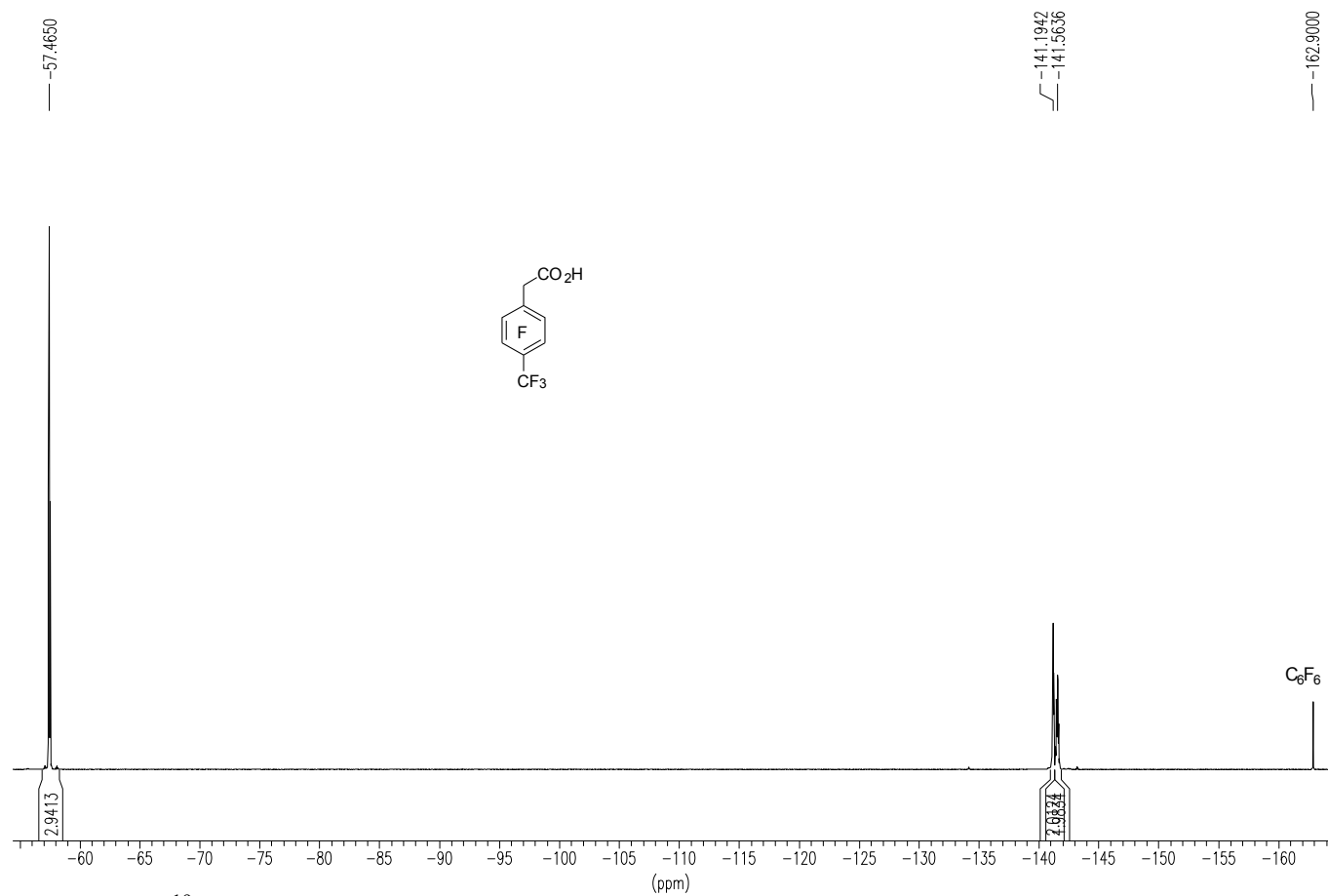


Figure S25. ¹⁹F NMR spectrum of **9d** (CDCl₃).

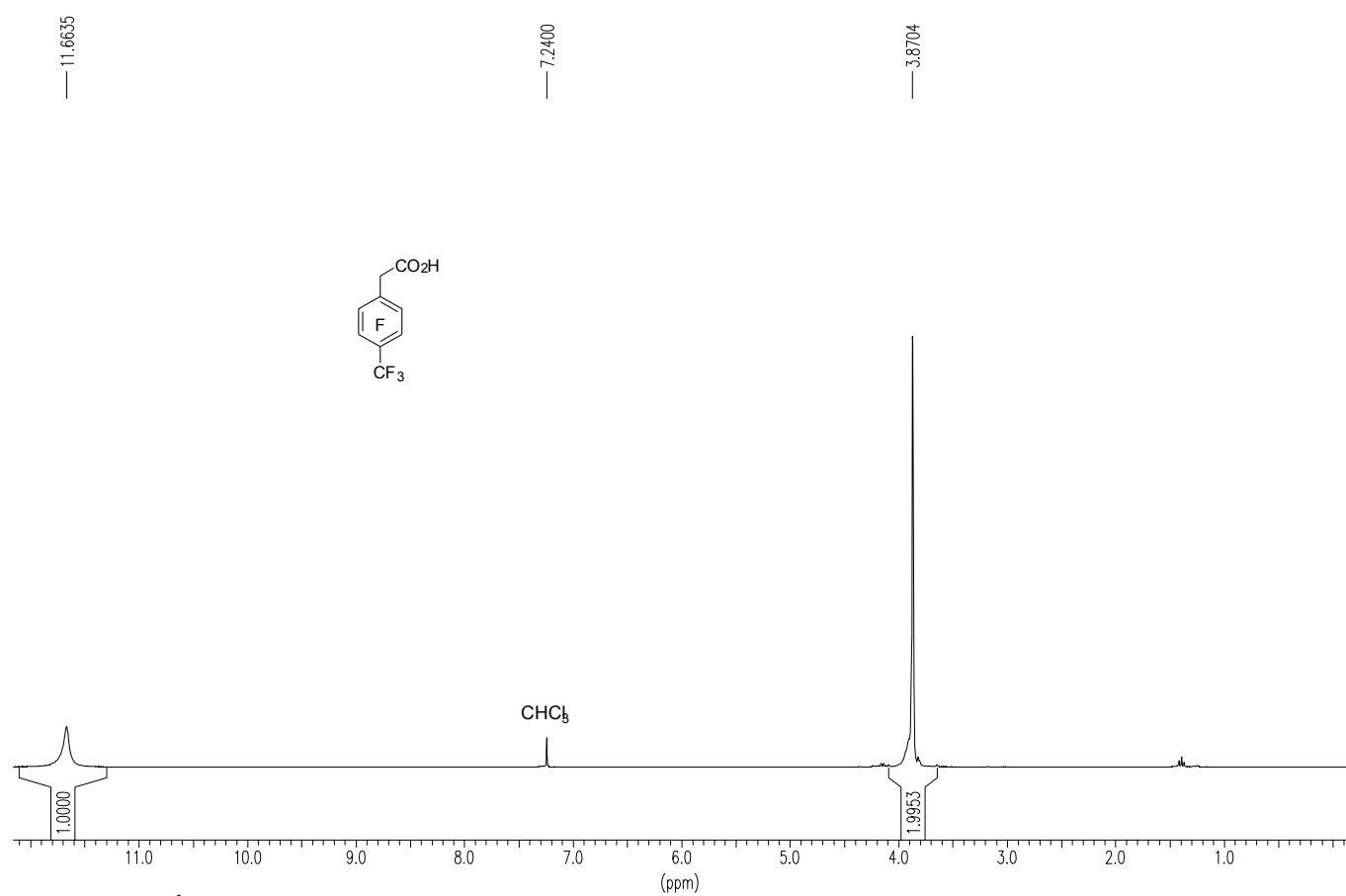


Figure S26. ¹H NMR spectrum of **9d** (CDCl₃).

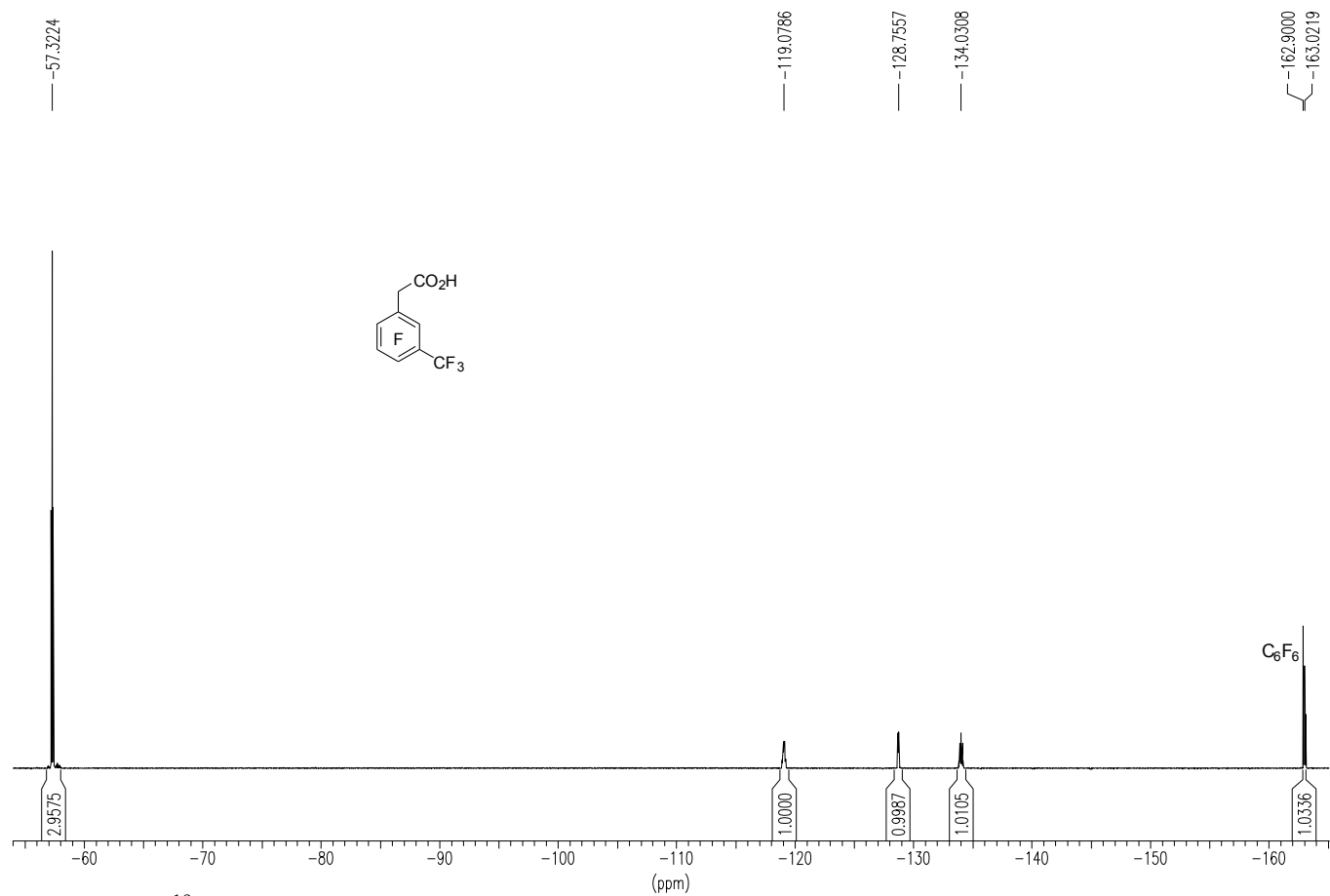


Figure S27. ^{19}F NMR spectrum of **9e** (CDCl_3).

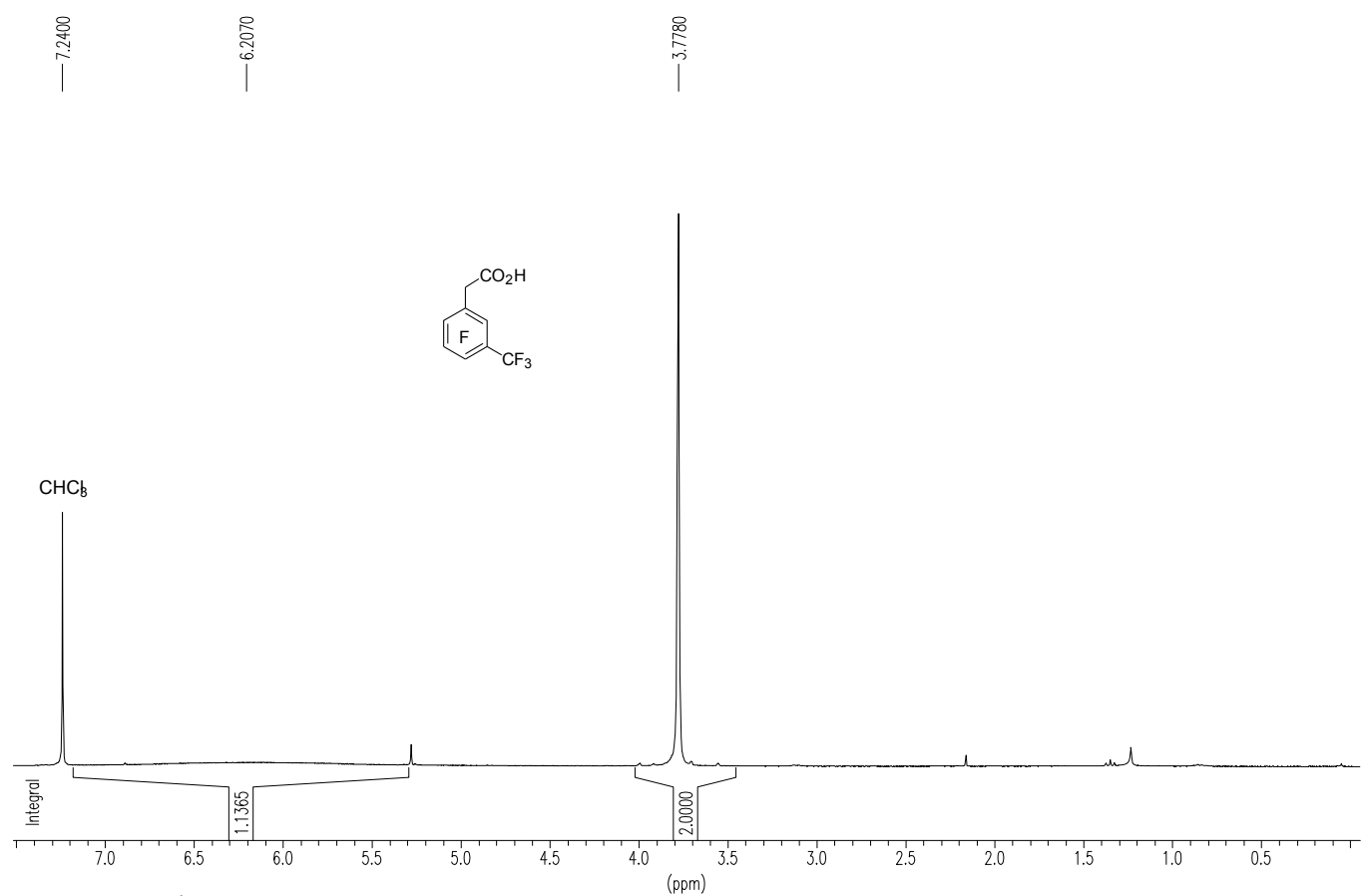


Figure S28. ^1H NMR spectrum of **9e** (CDCl_3).

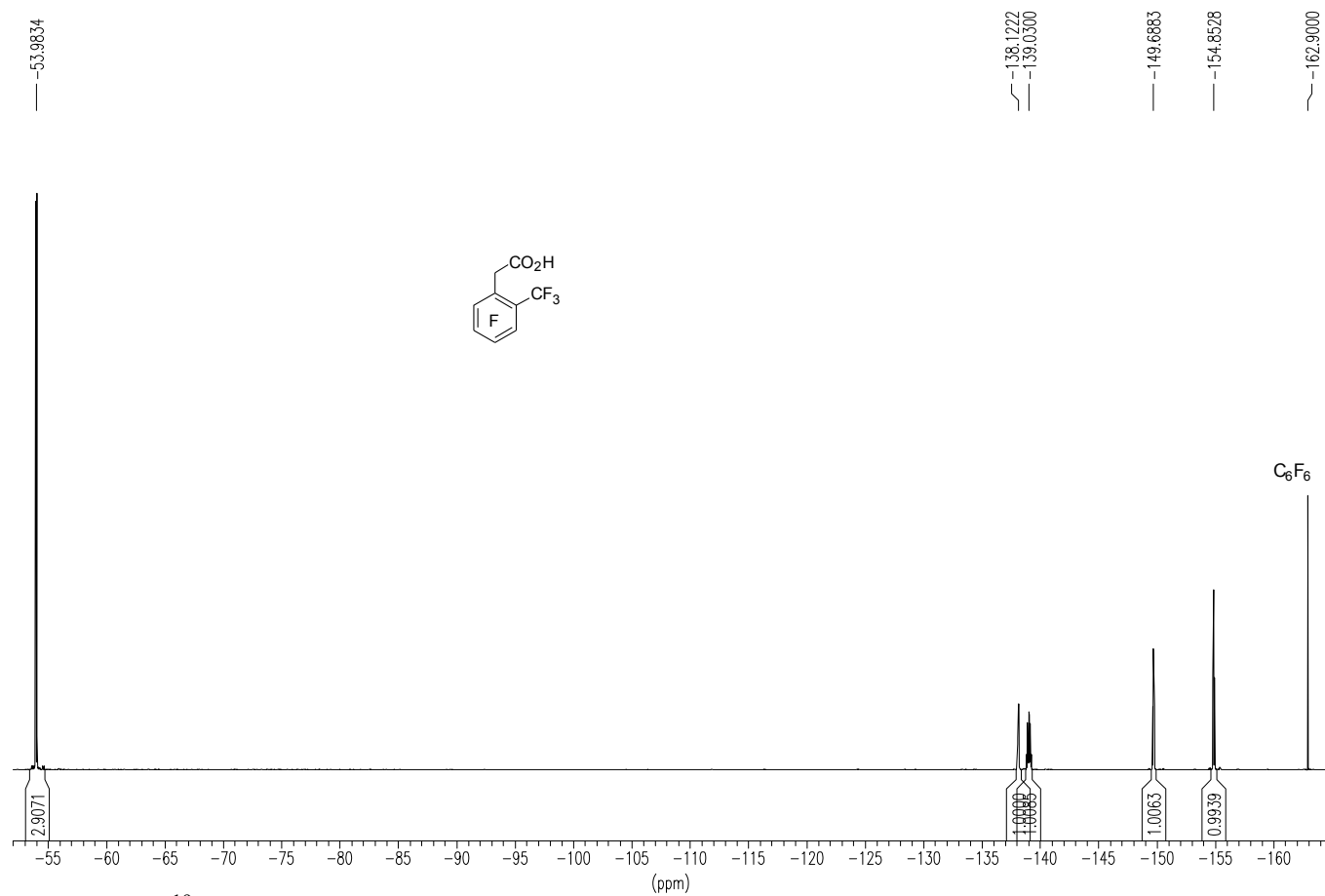


Figure S29. ¹⁹F NMR spectrum of **9f** (acetone-*d*₆).

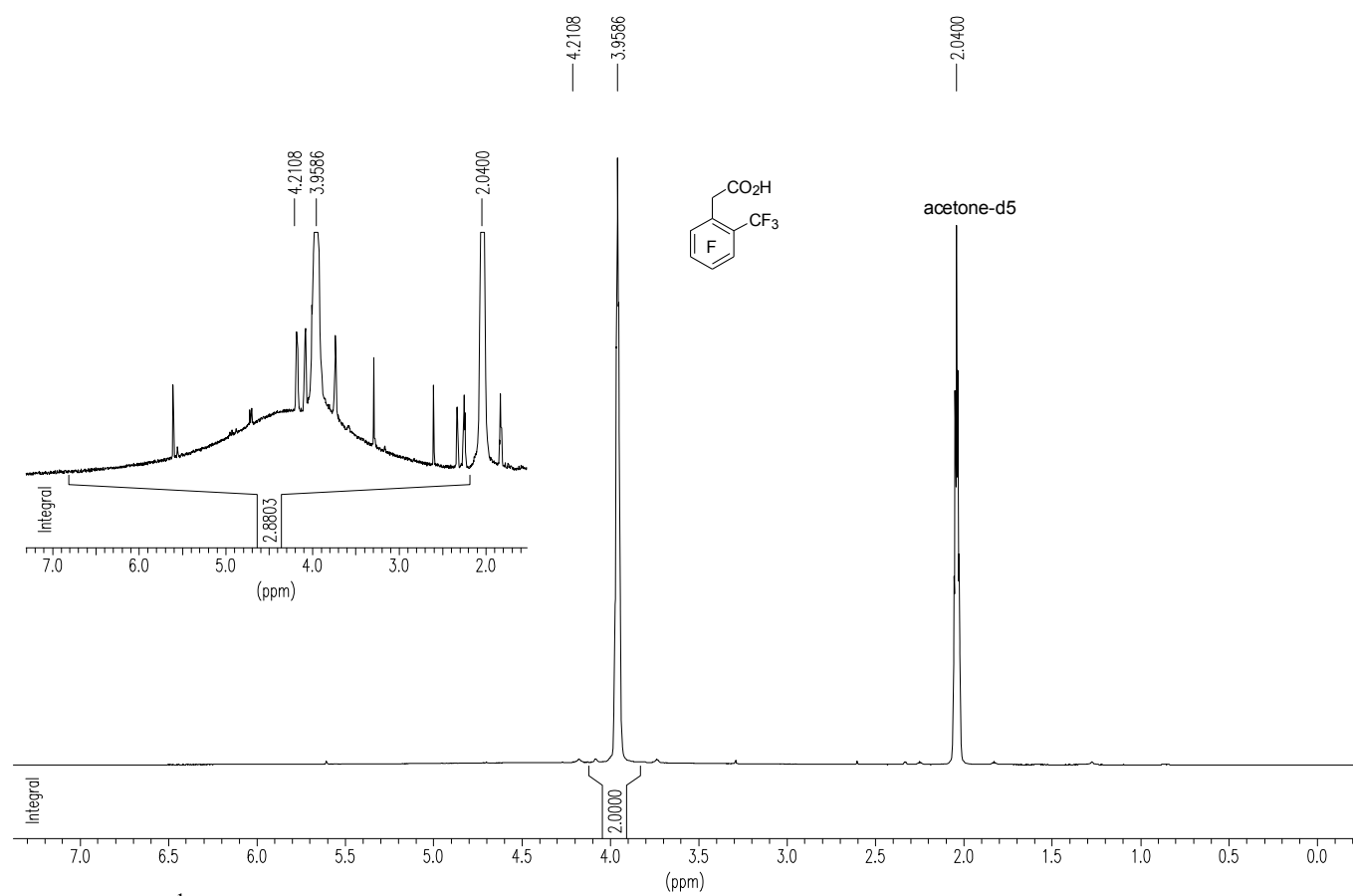


Figure S30. ¹H NMR spectrum of **9f** (acetone-*d*₆).

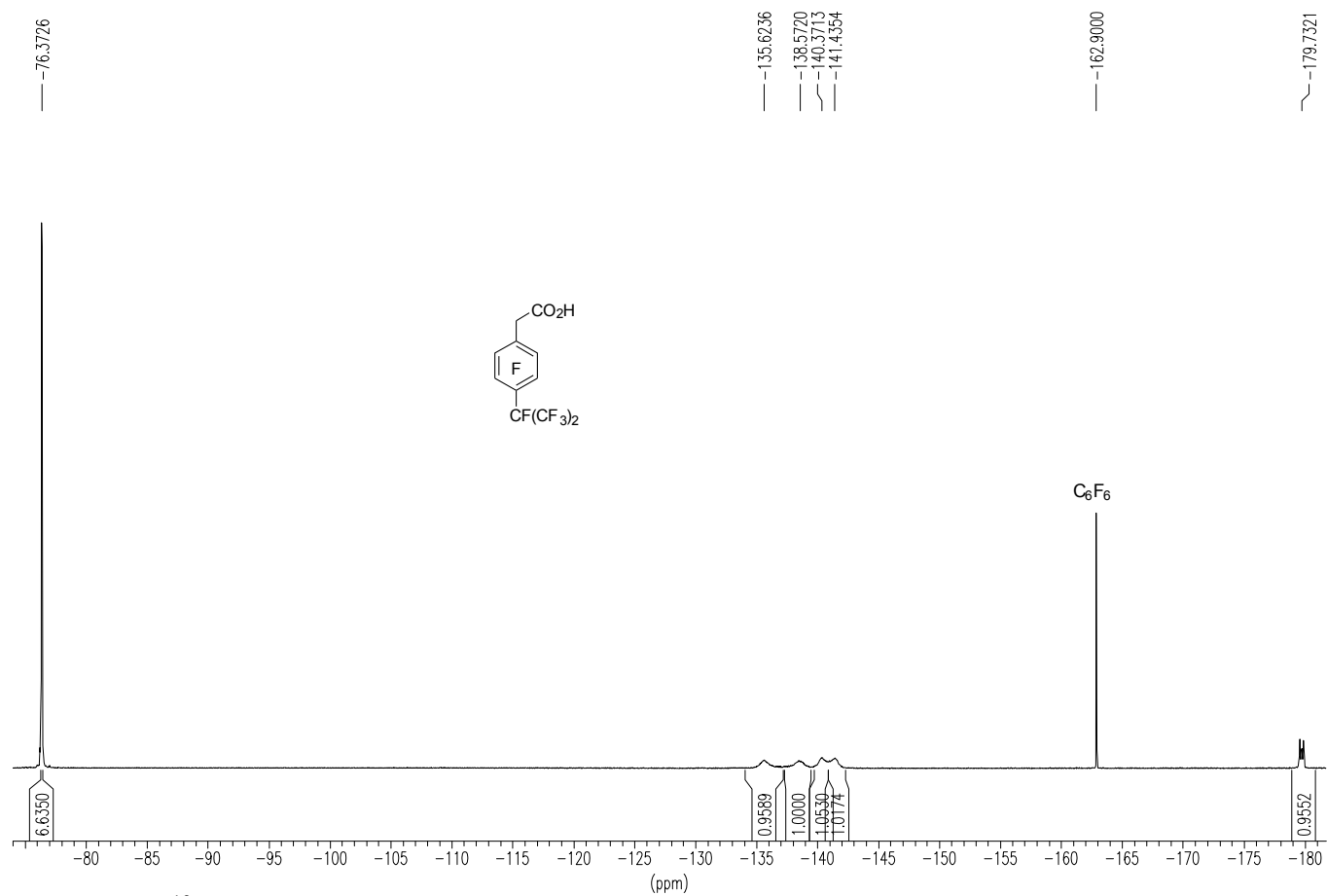


Figure S31. ¹⁹F NMR spectrum of **9g** (CDCl₃).

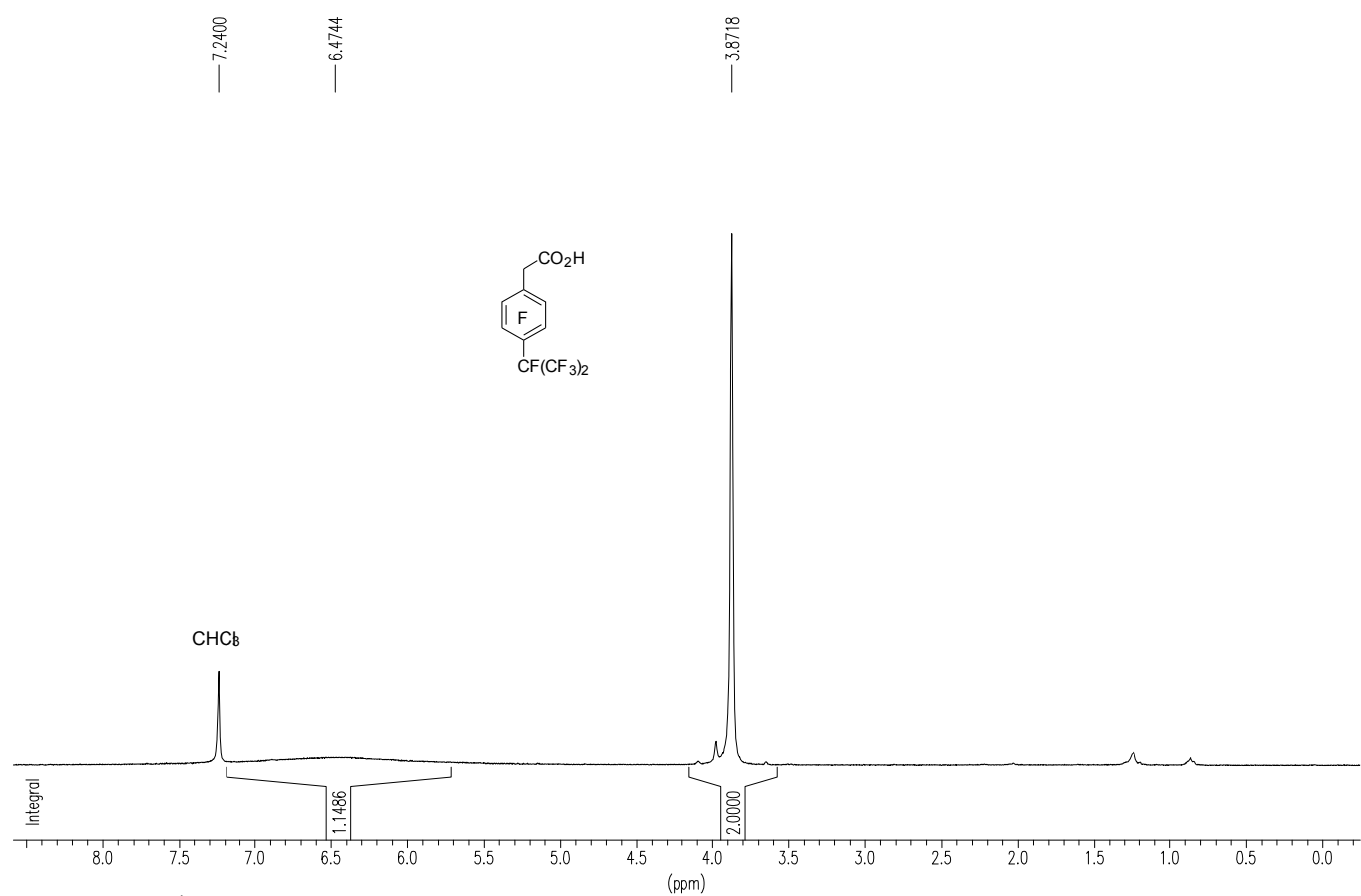


Figure S32. ¹H NMR spectrum of **9g** (CDCl₃).

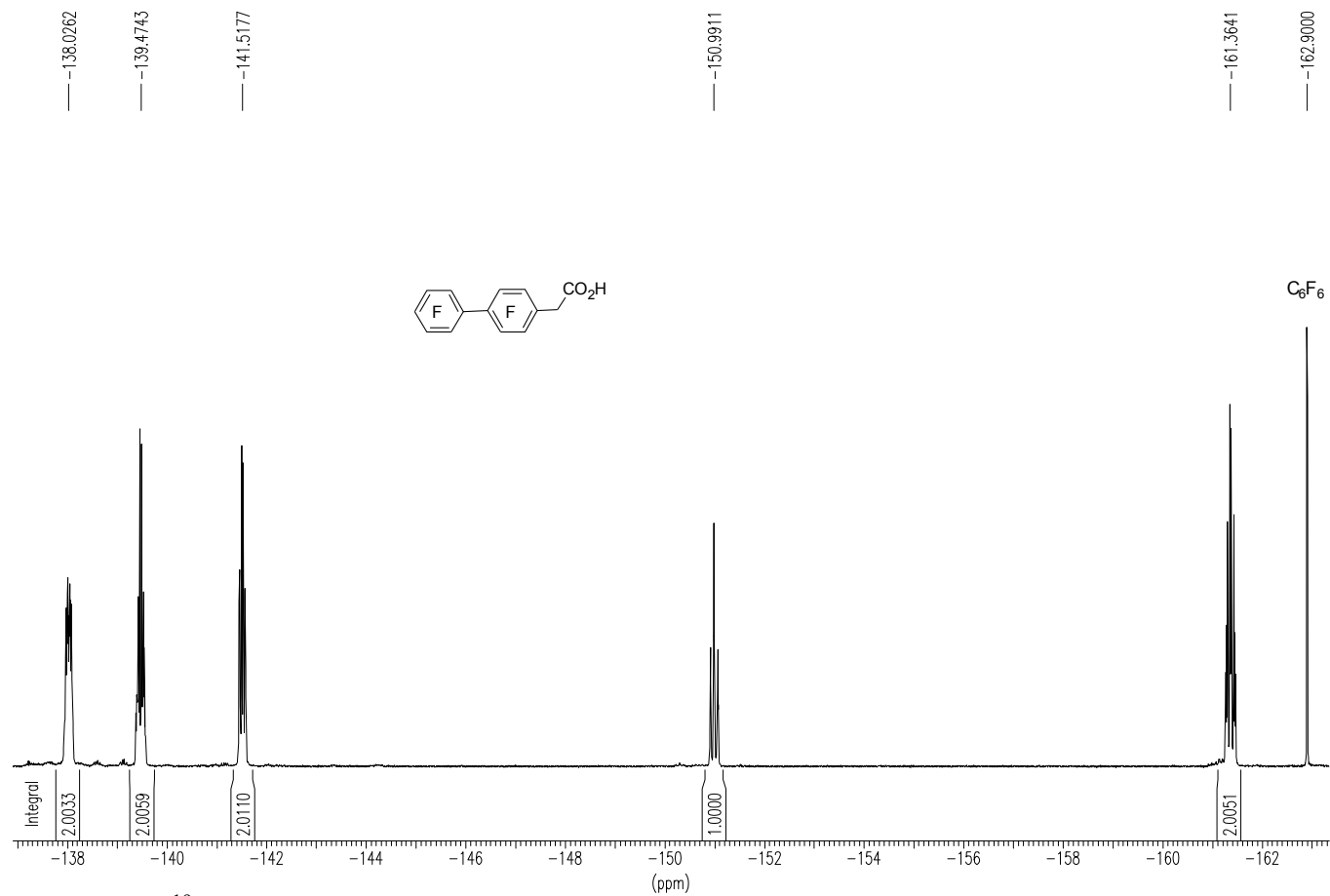


Figure S33. ¹⁹F NMR spectrum of **9h** (acetone-*d*₆).

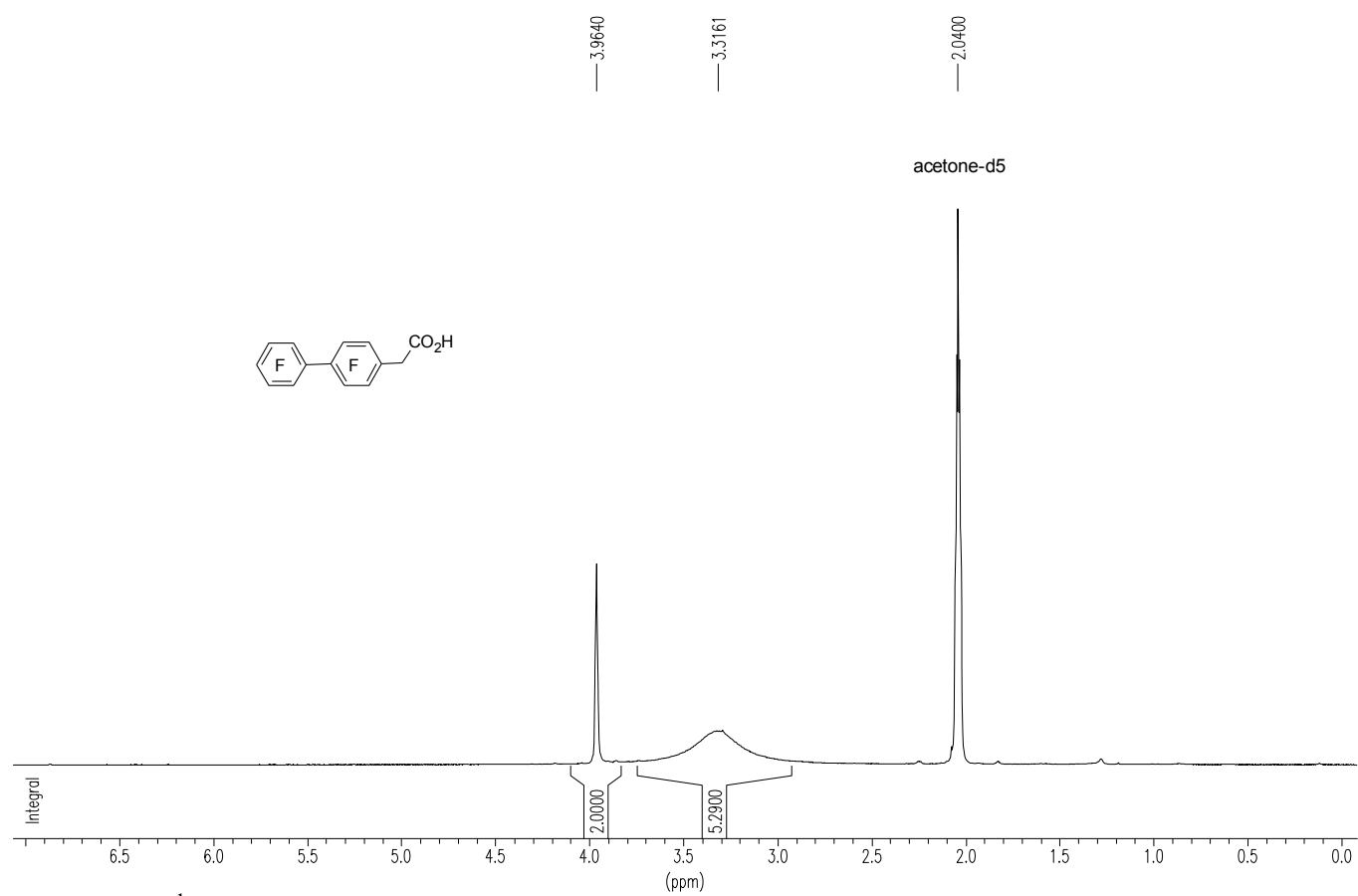


Figure S34. ¹H NMR spectrum of **9h** (acetone-*d*₆).

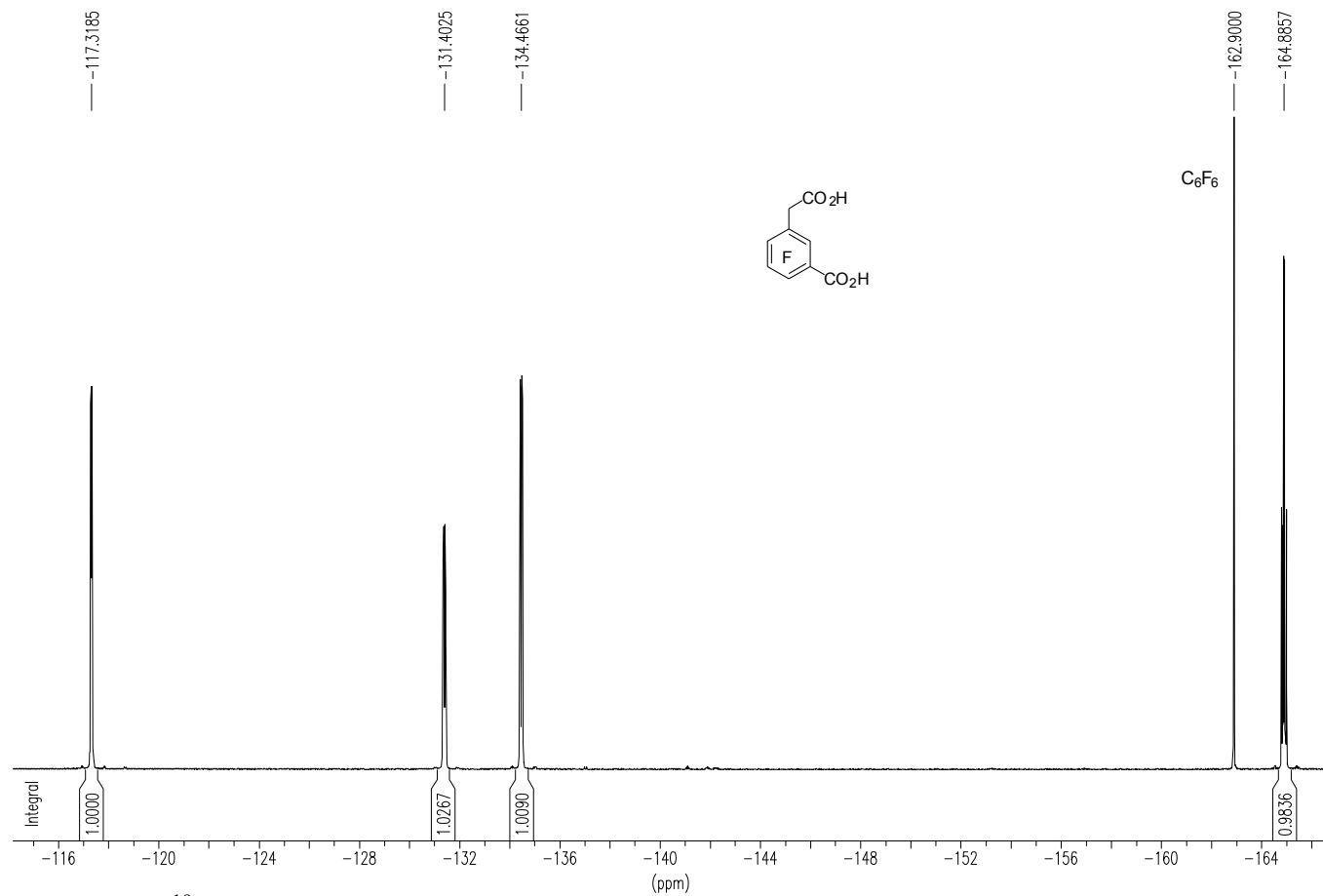


Figure S35. ^{19}F NMR spectrum of **11** (acetone- d_6).

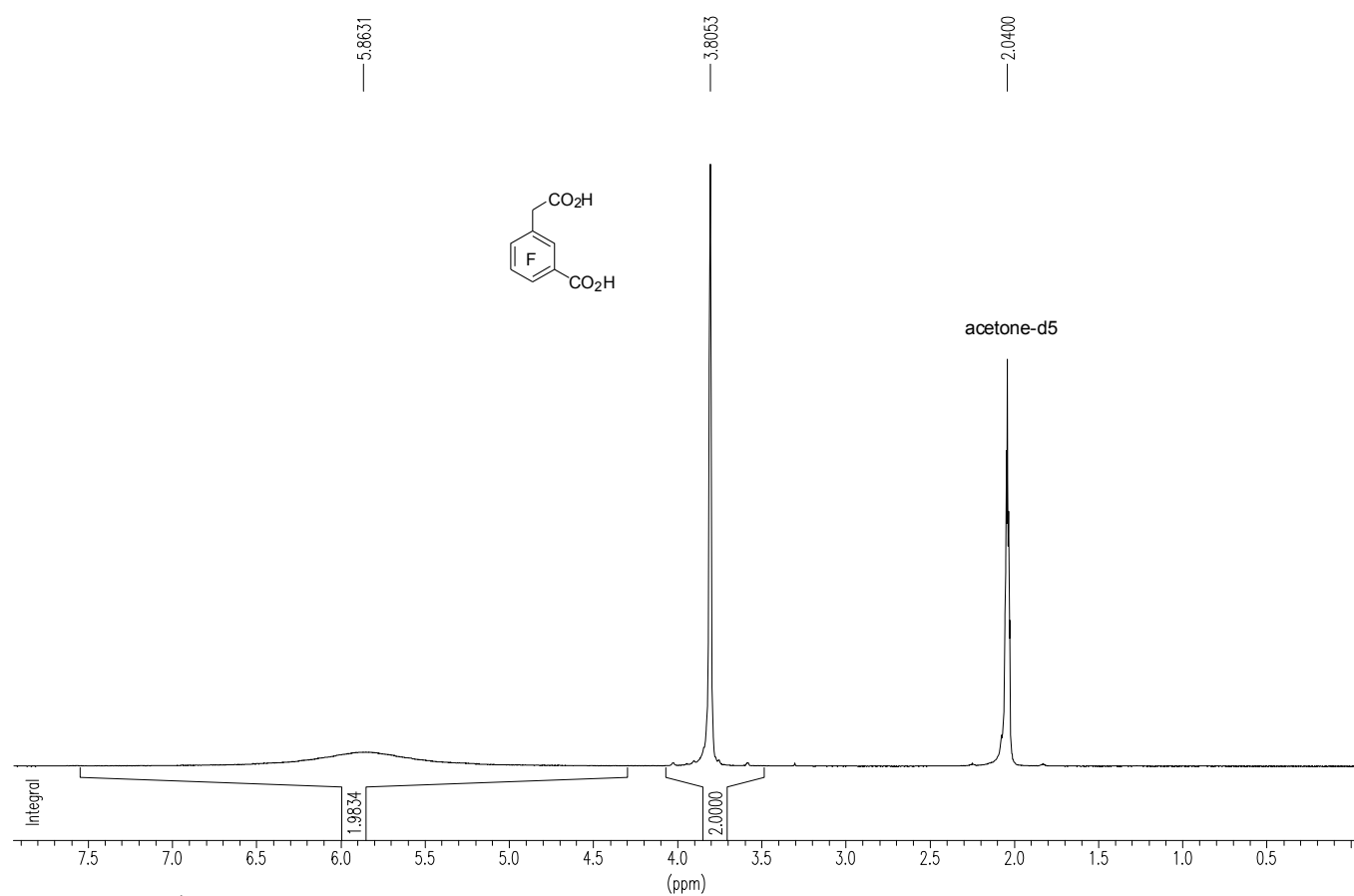


Figure S36. ^1H NMR spectrum of **11** (acetone- d_6).

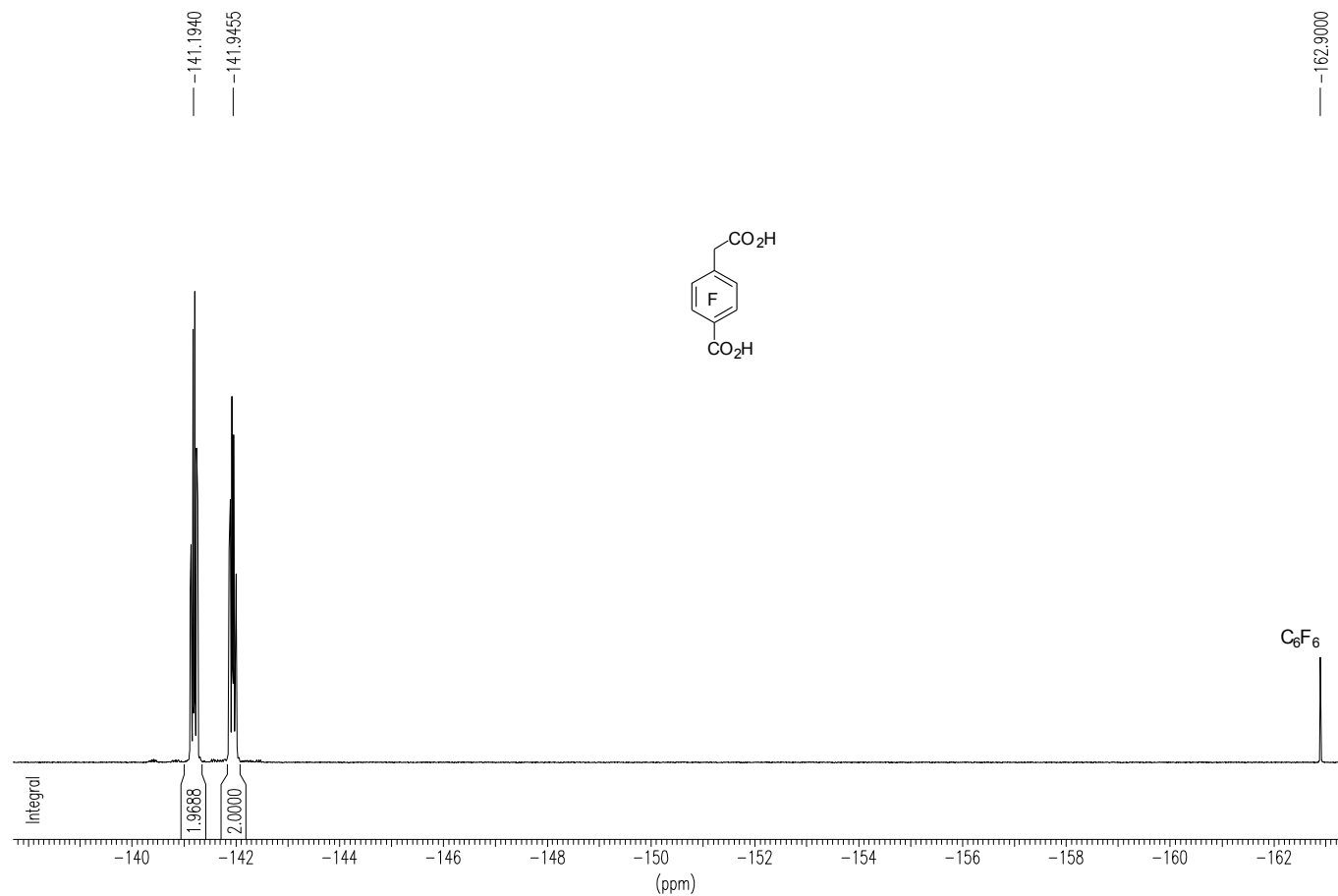


Figure S37. ¹⁹F NMR spectrum of **12** (acetone-*d*₆).

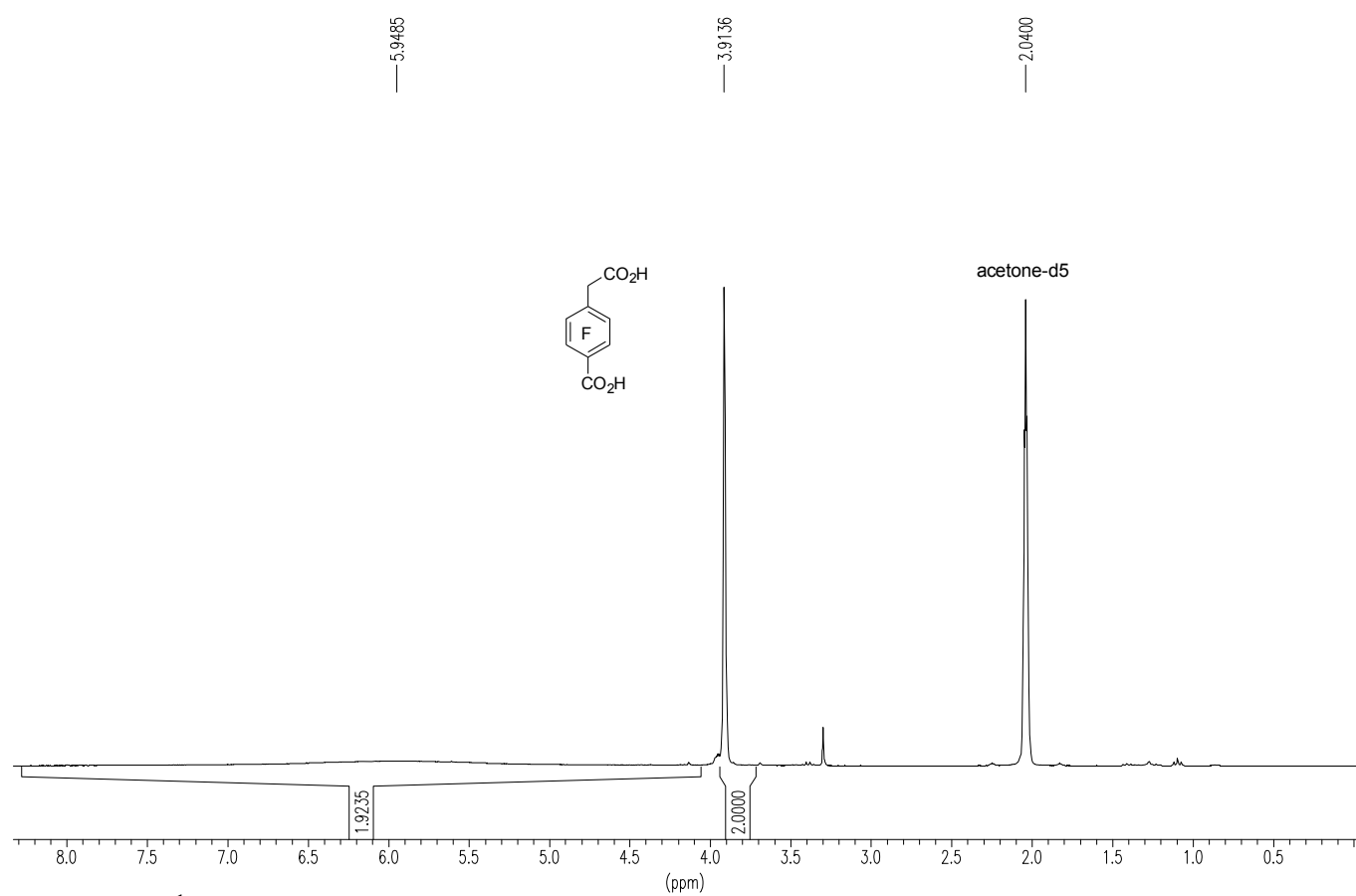


Figure S38. ¹H NMR spectrum of **12** (acetone-*d*₆).

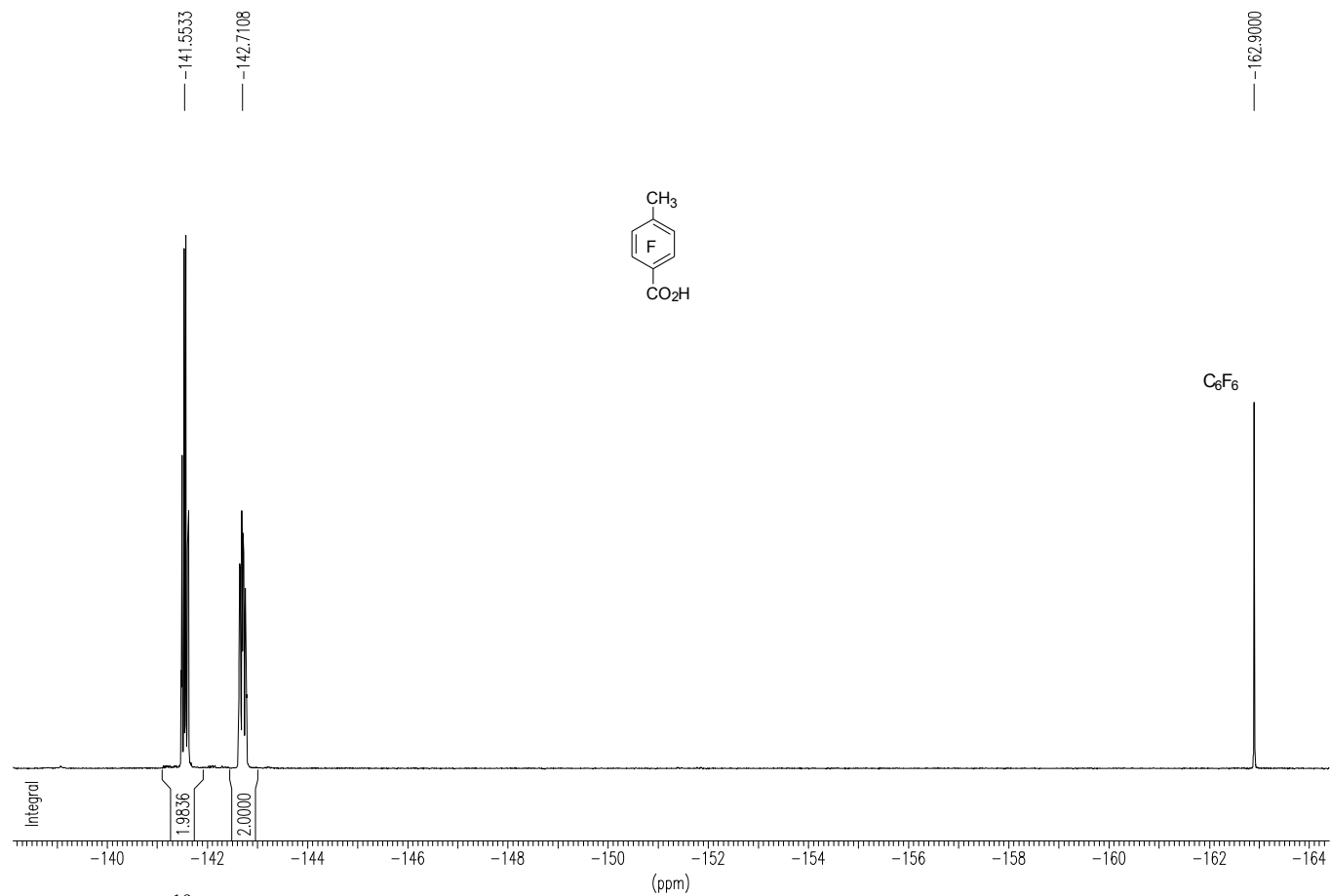


Figure S39. ¹⁹F NMR spectrum of **13** (acetone-*d*₆).

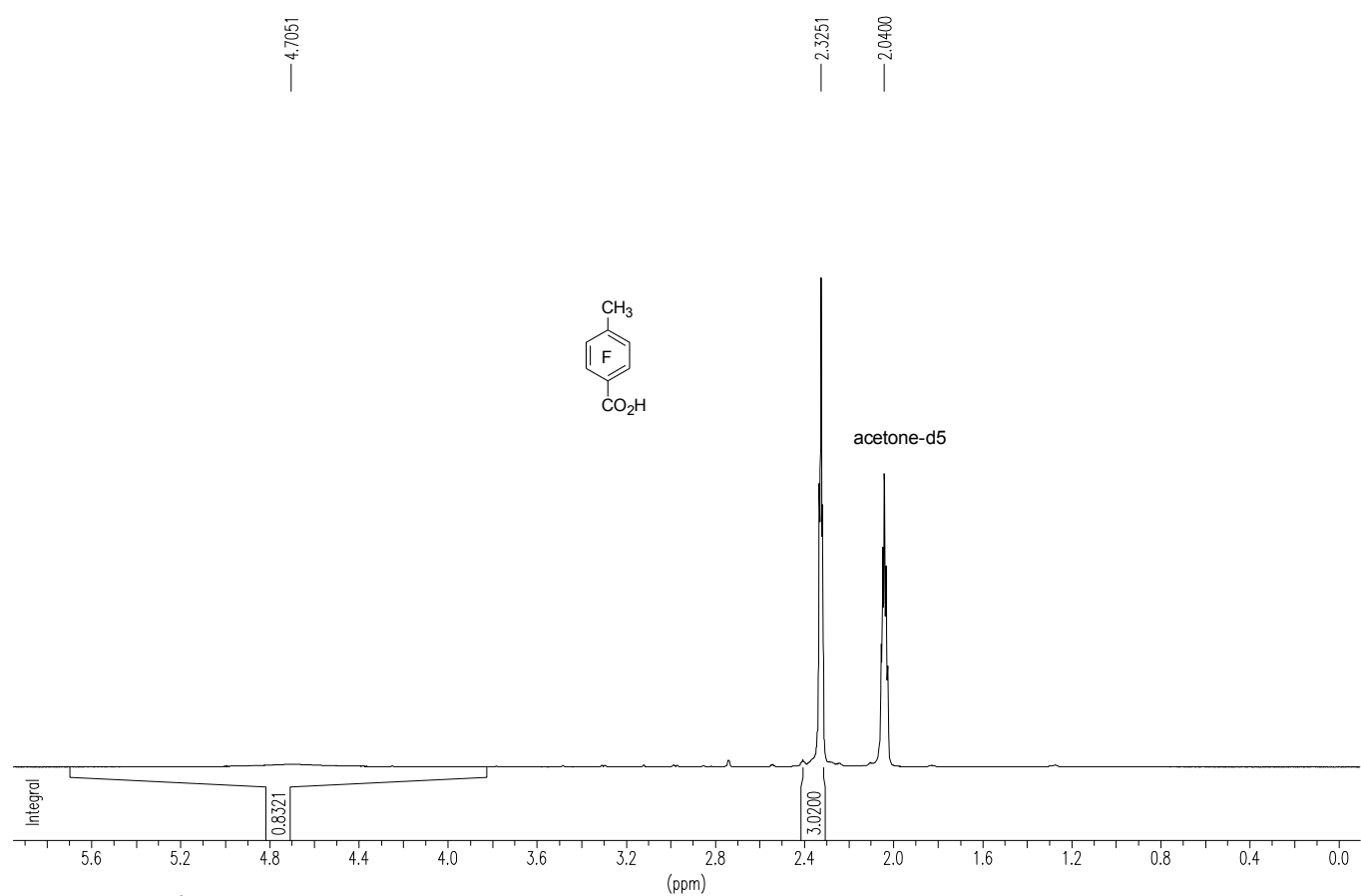


Figure S40. ¹H NMR spectrum of **13** (acetone-*d*₆).

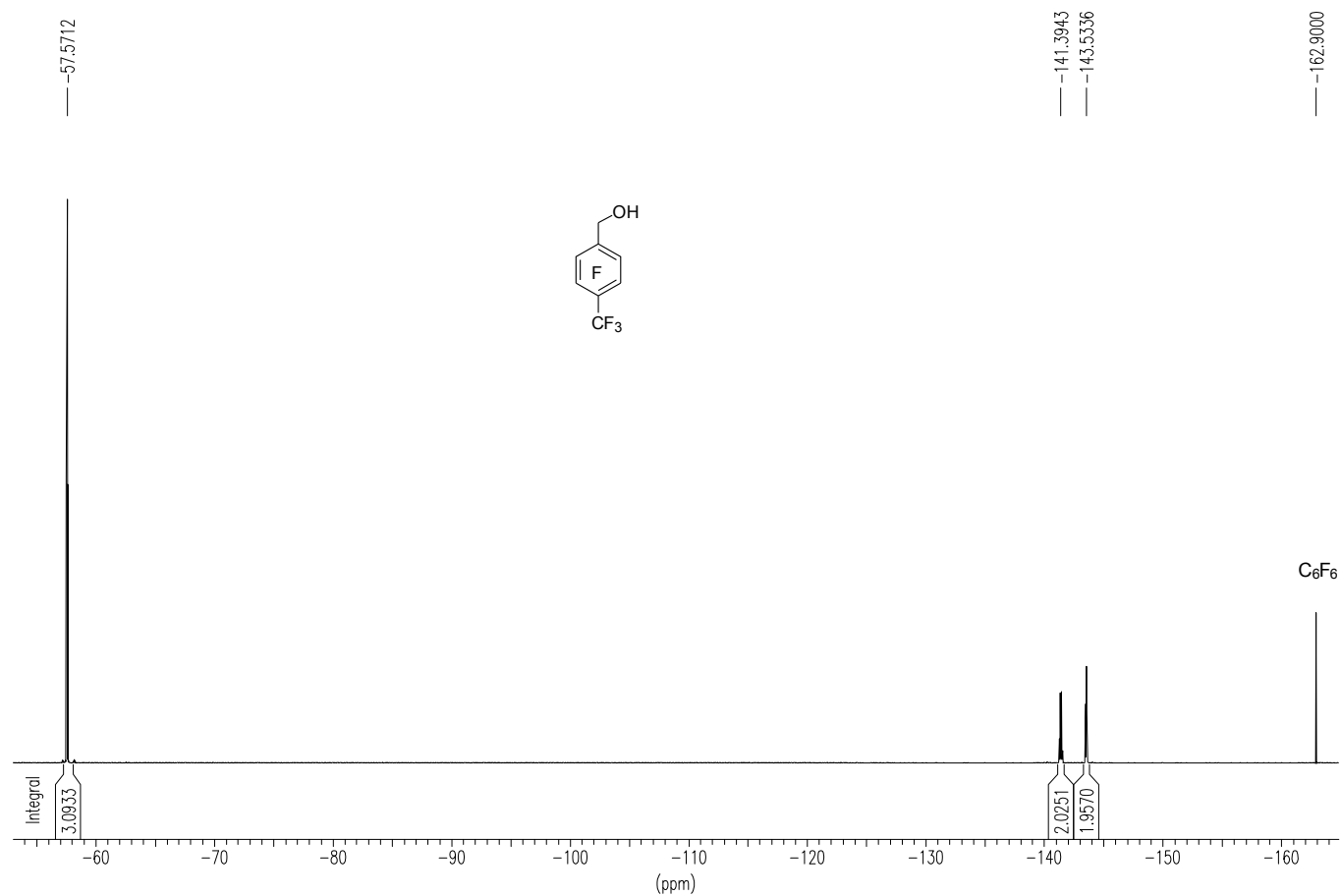


Figure S41. ¹⁹F NMR spectrum of **14d** (CDCl₃).

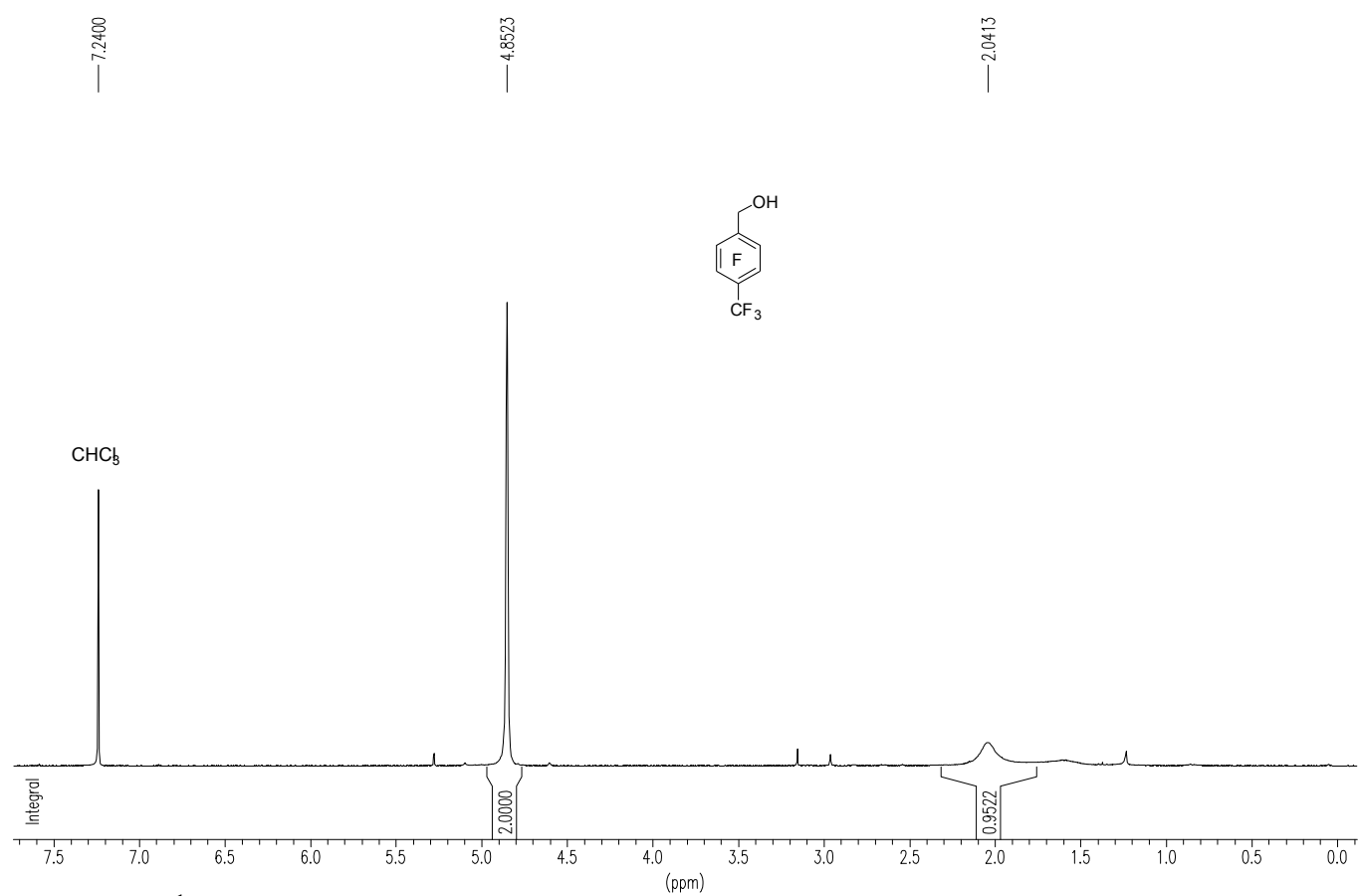


Figure S42. ¹H NMR spectrum of **14d** (CDCl₃).

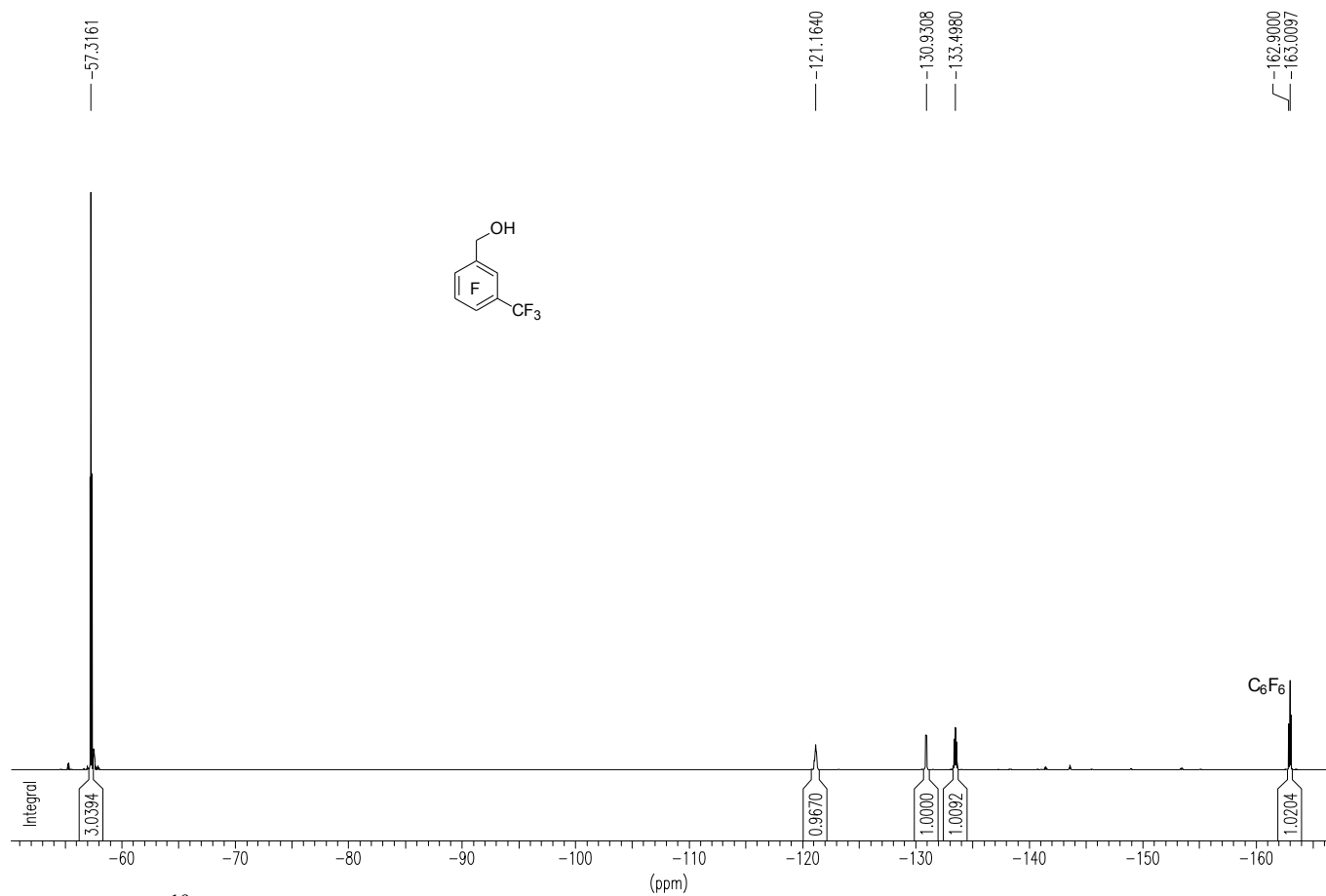


Figure S43. ^{19}F NMR spectrum of **14e** (CDCl_3).

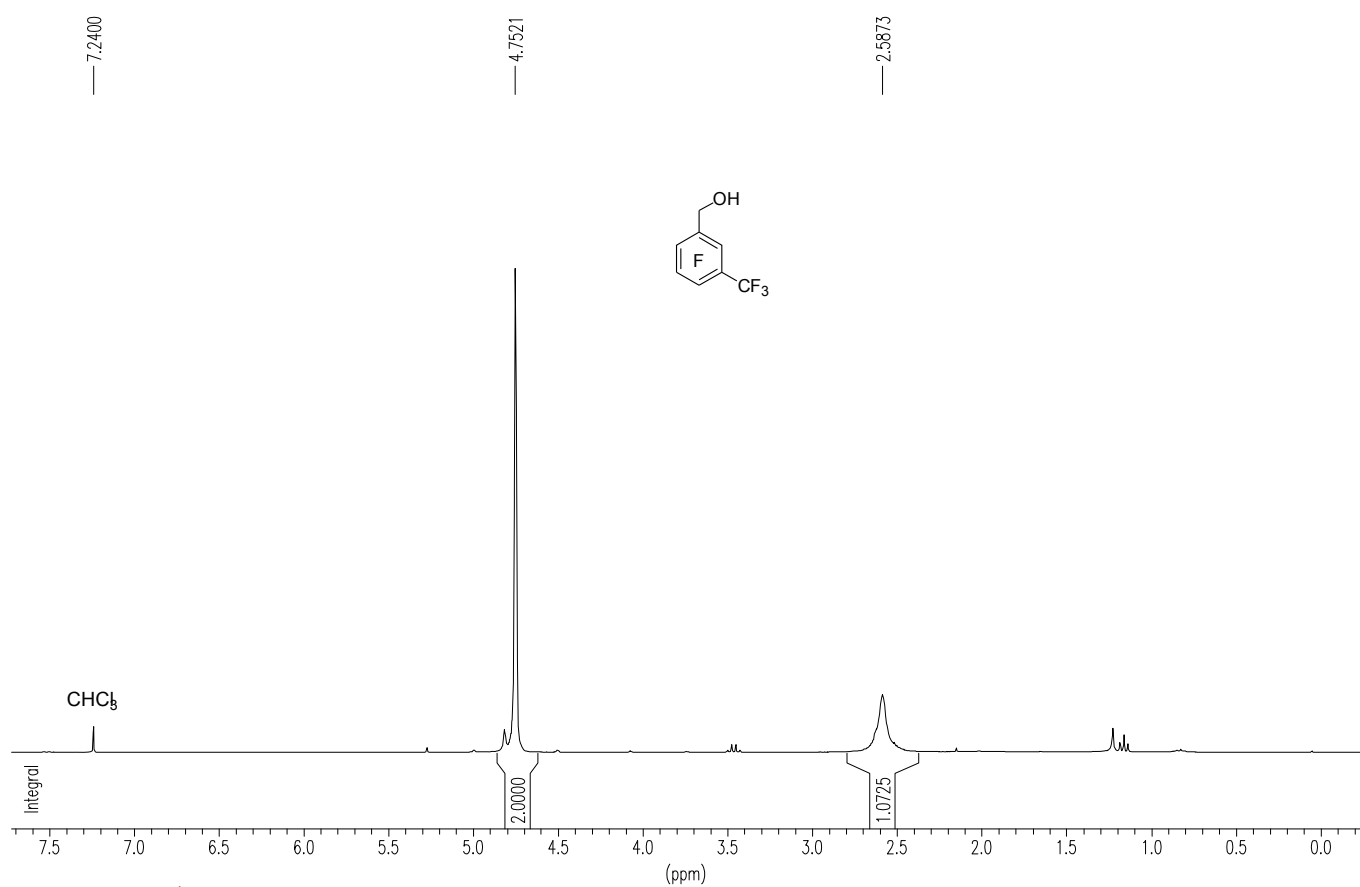


Figure S44. ^1H NMR spectrum of **14e** (CDCl_3).

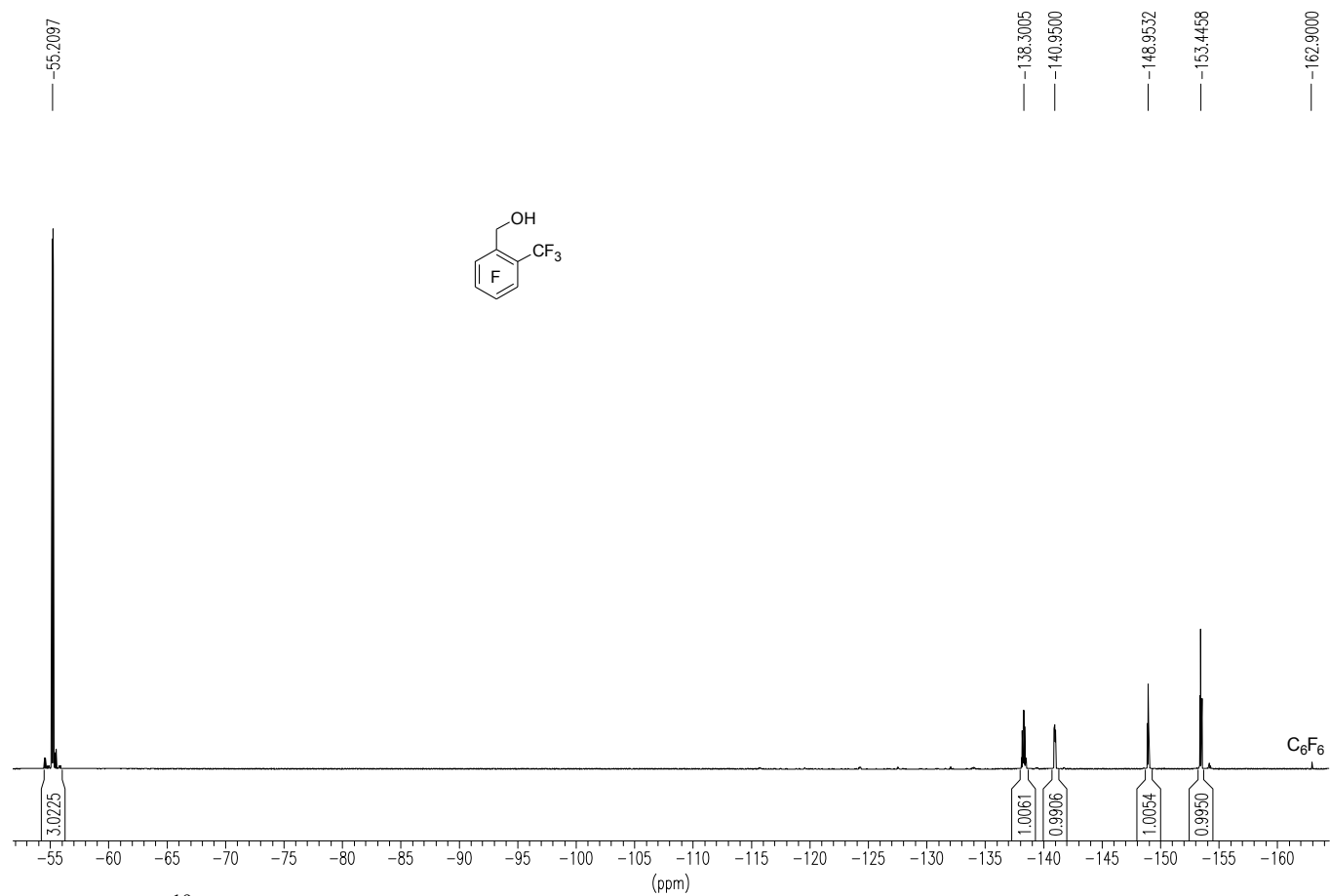


Figure S45. ¹⁹F NMR spectrum of **14f** (CDCl₃).

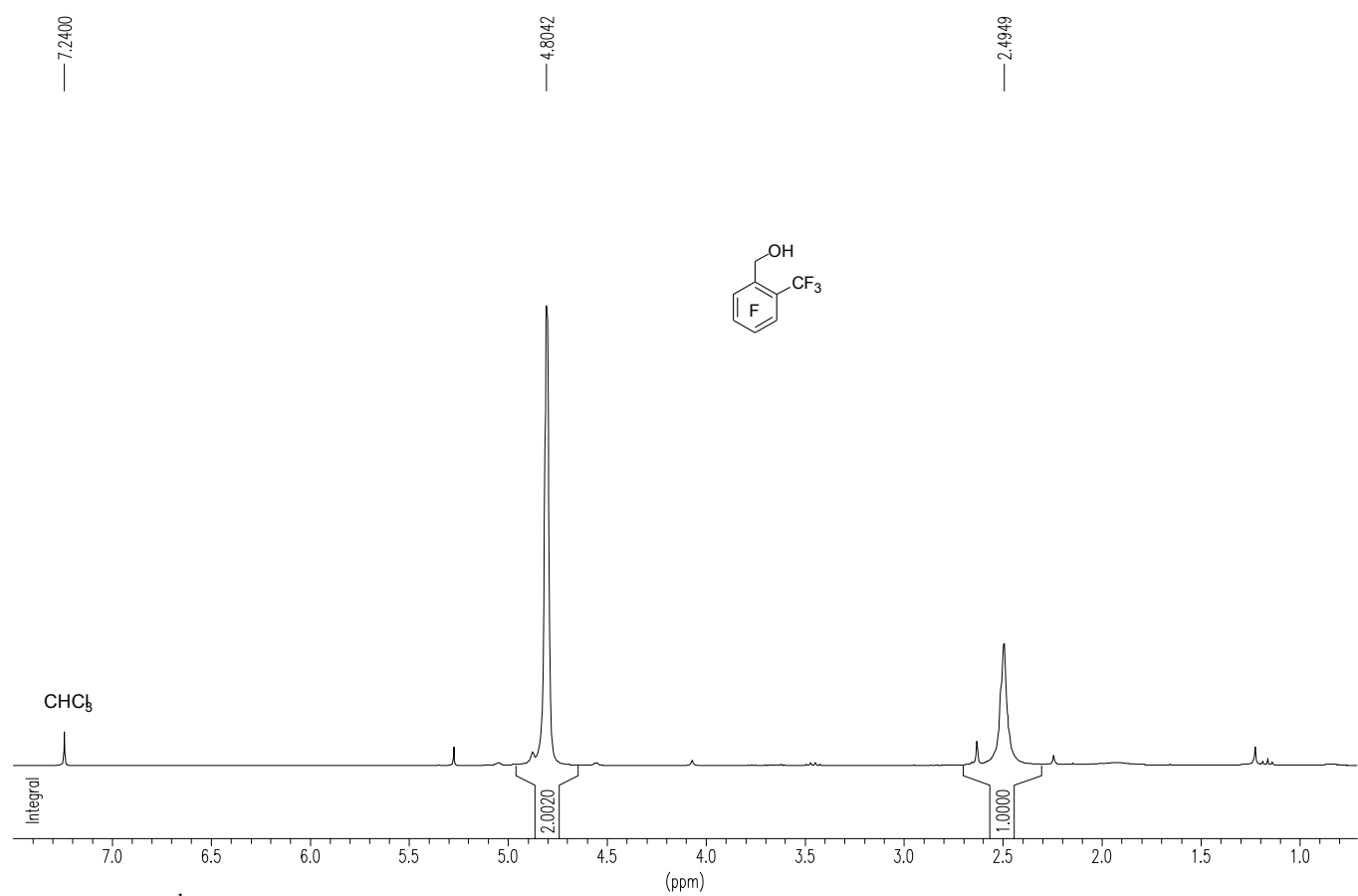


Figure S46. ¹H NMR spectrum of **14f** (CDCl₃).

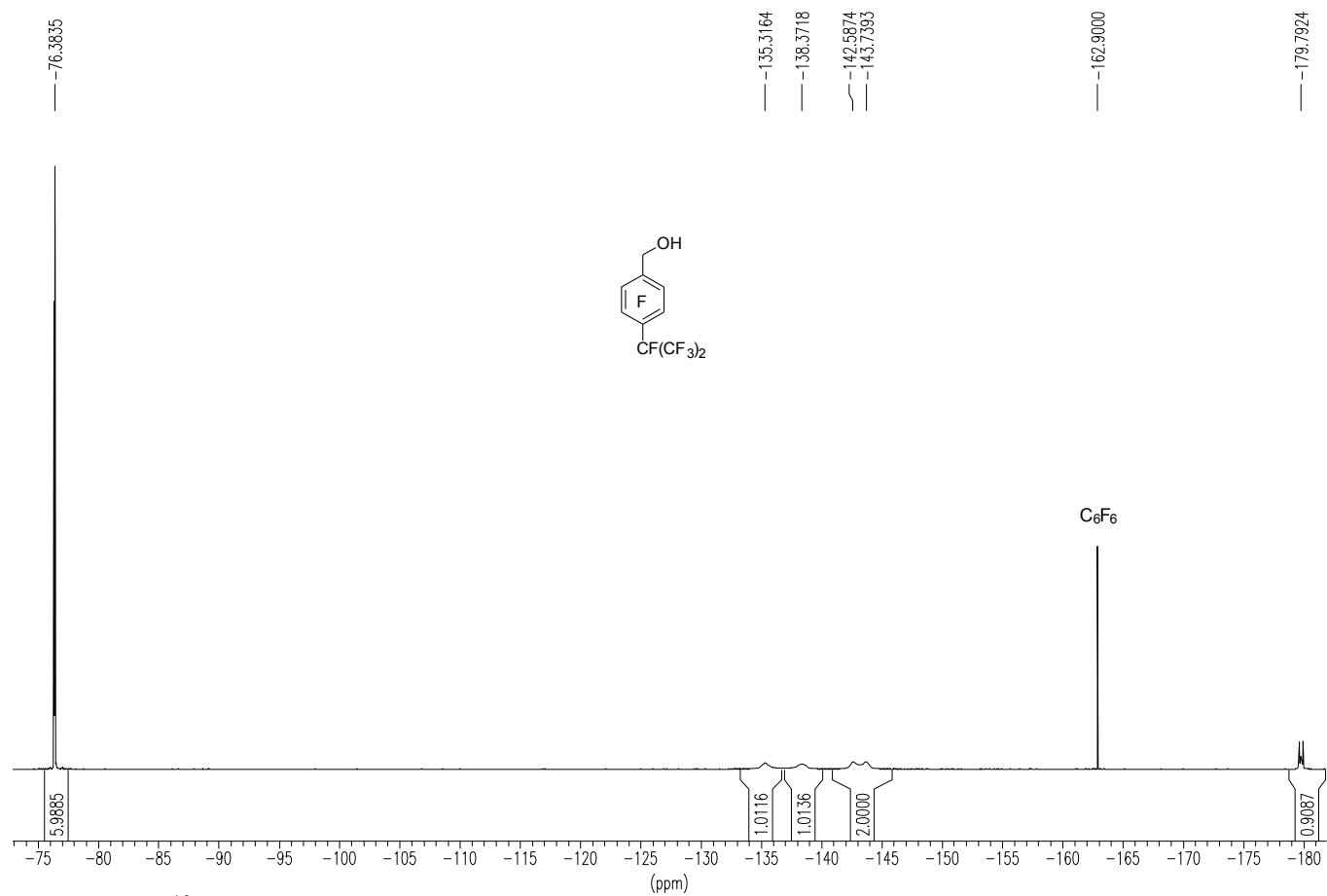


Figure S47. ¹⁹F NMR spectrum of **14g** (CDCl₃).

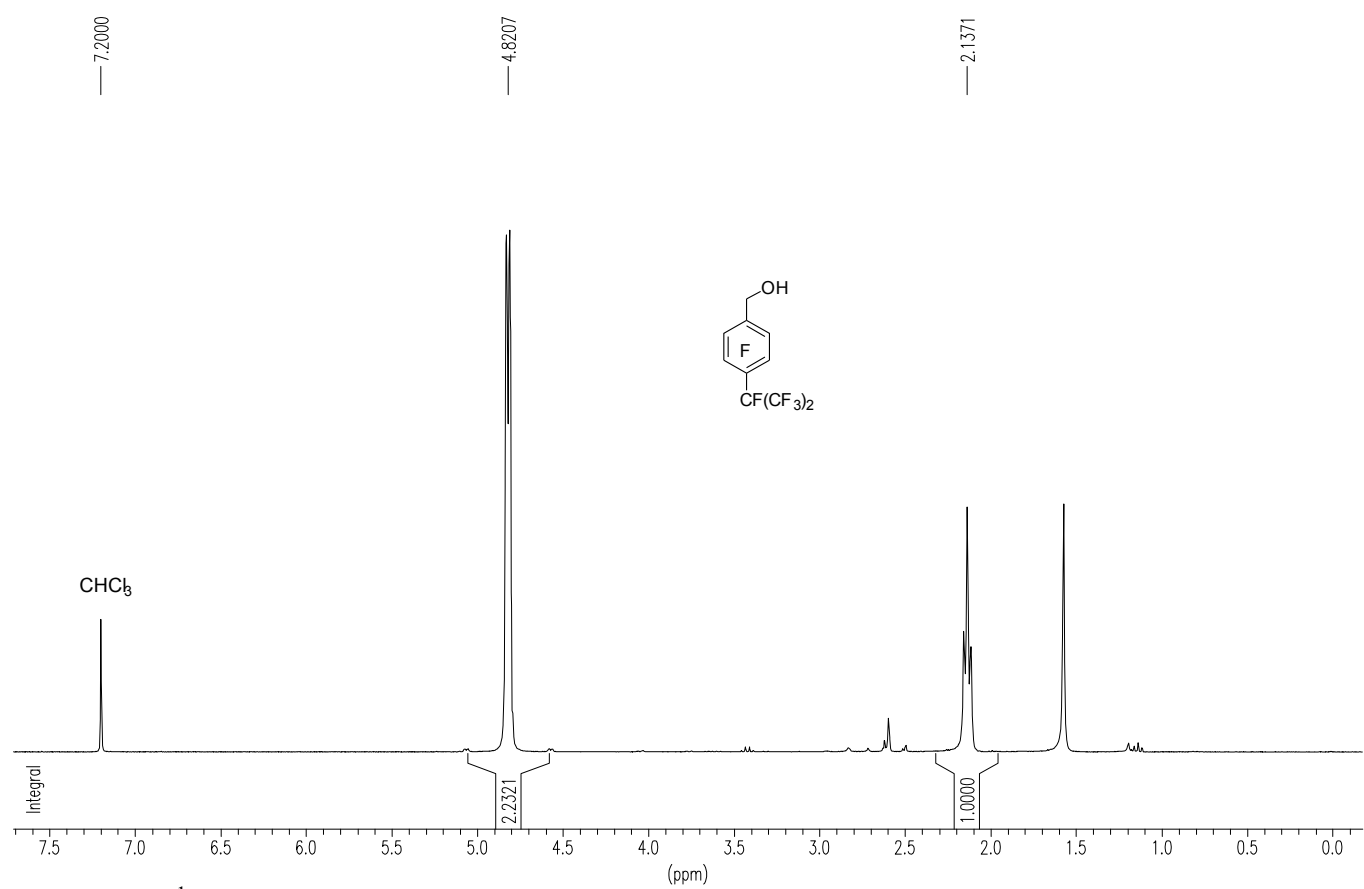


Figure S48. ¹H NMR spectrum of **14g** (CDCl₃).

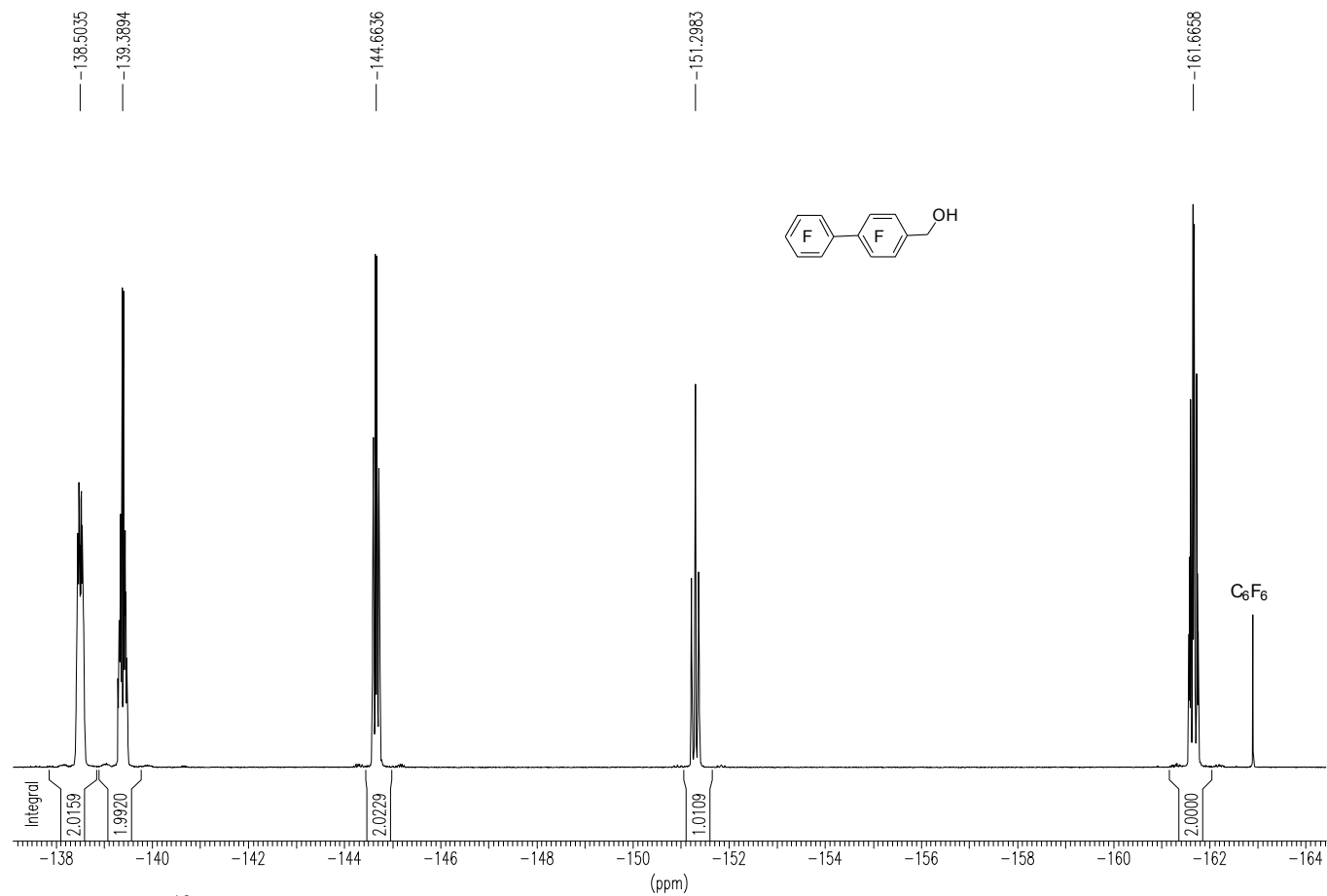


Figure S49. ^{19}F NMR spectrum of **14h** (CDCl_3).

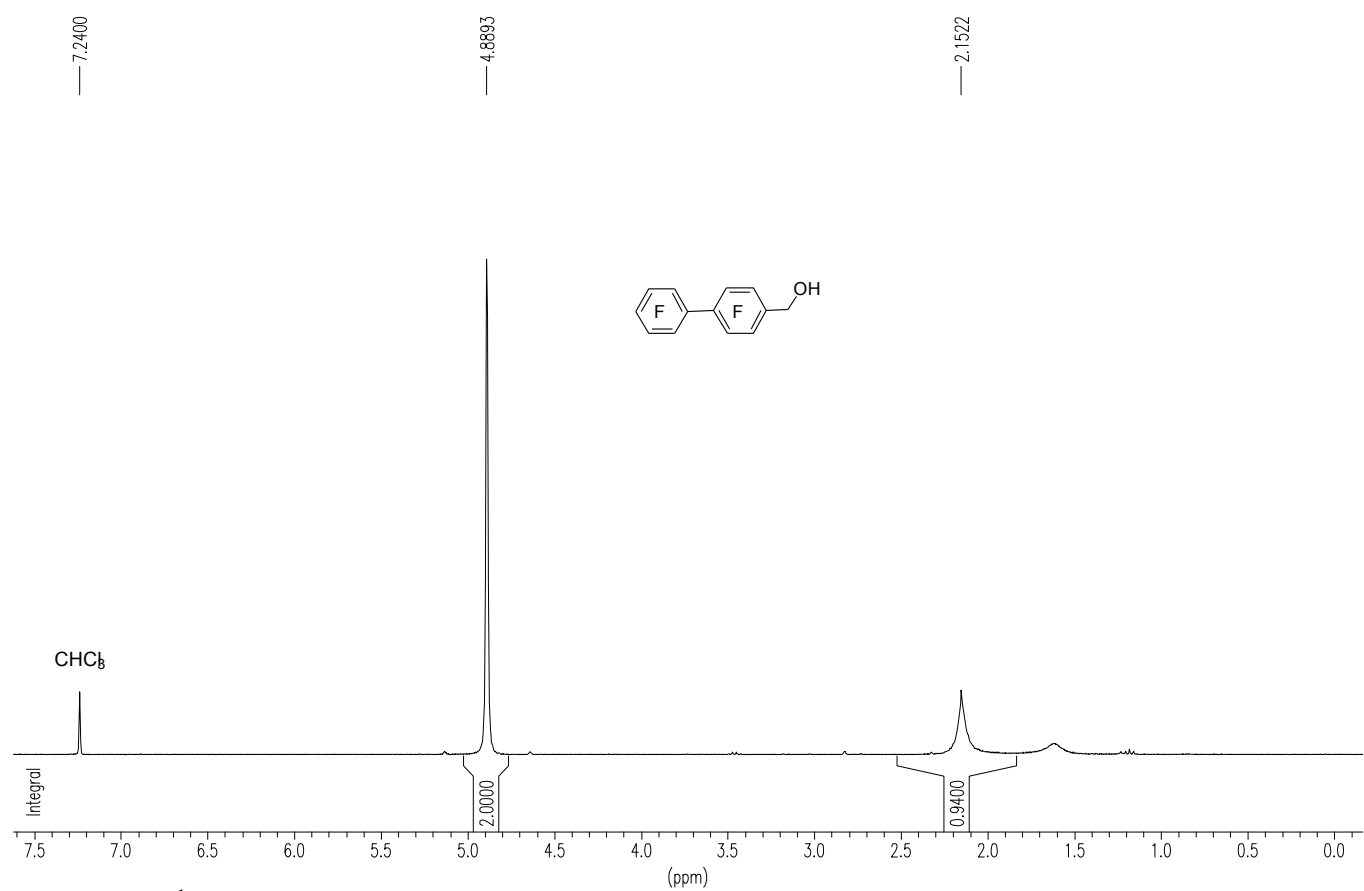


Figure S50. ^1H NMR spectrum of **14h** (CDCl_3).

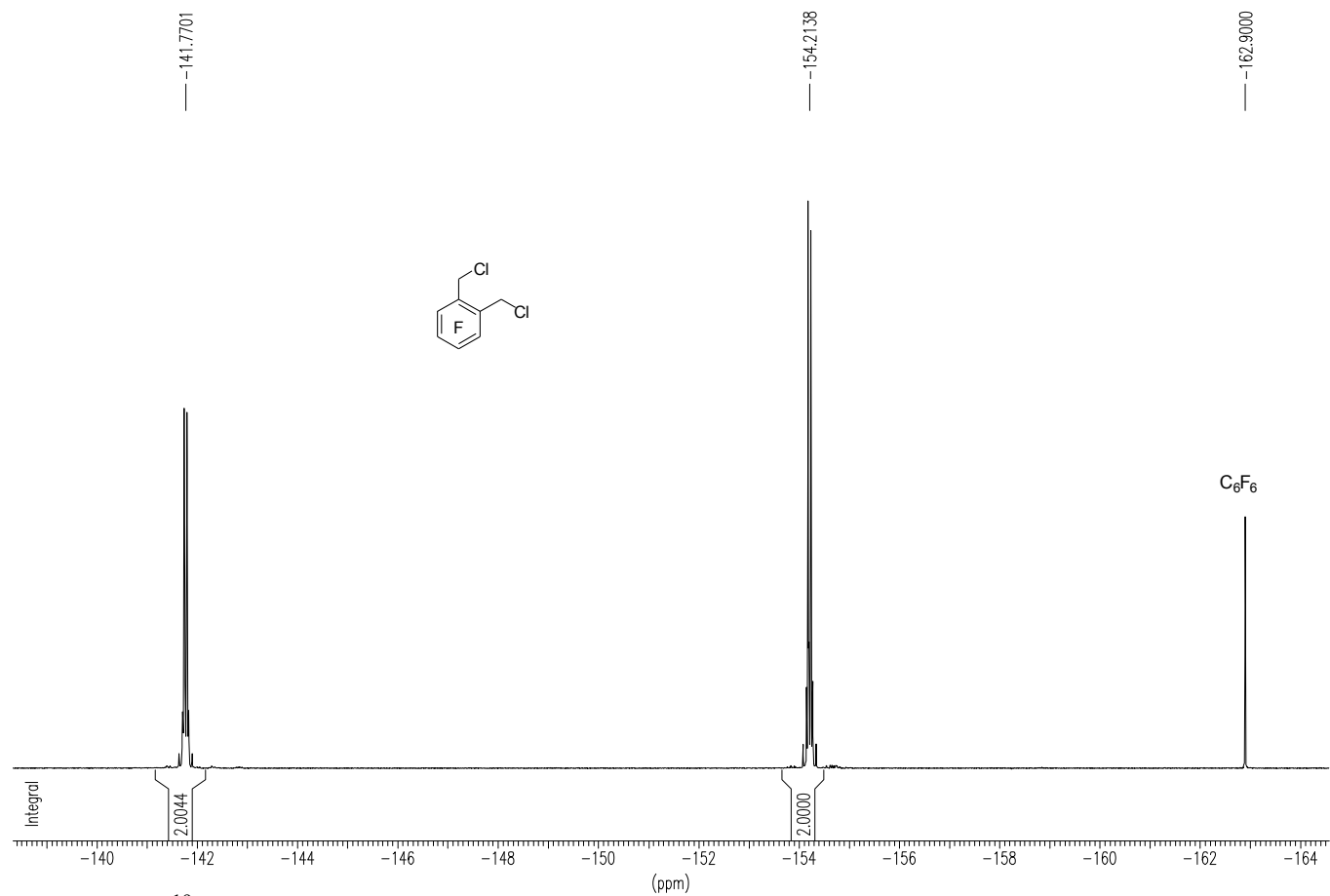


Figure S51. ¹⁹F NMR spectrum of **16c** (CDCl₃).

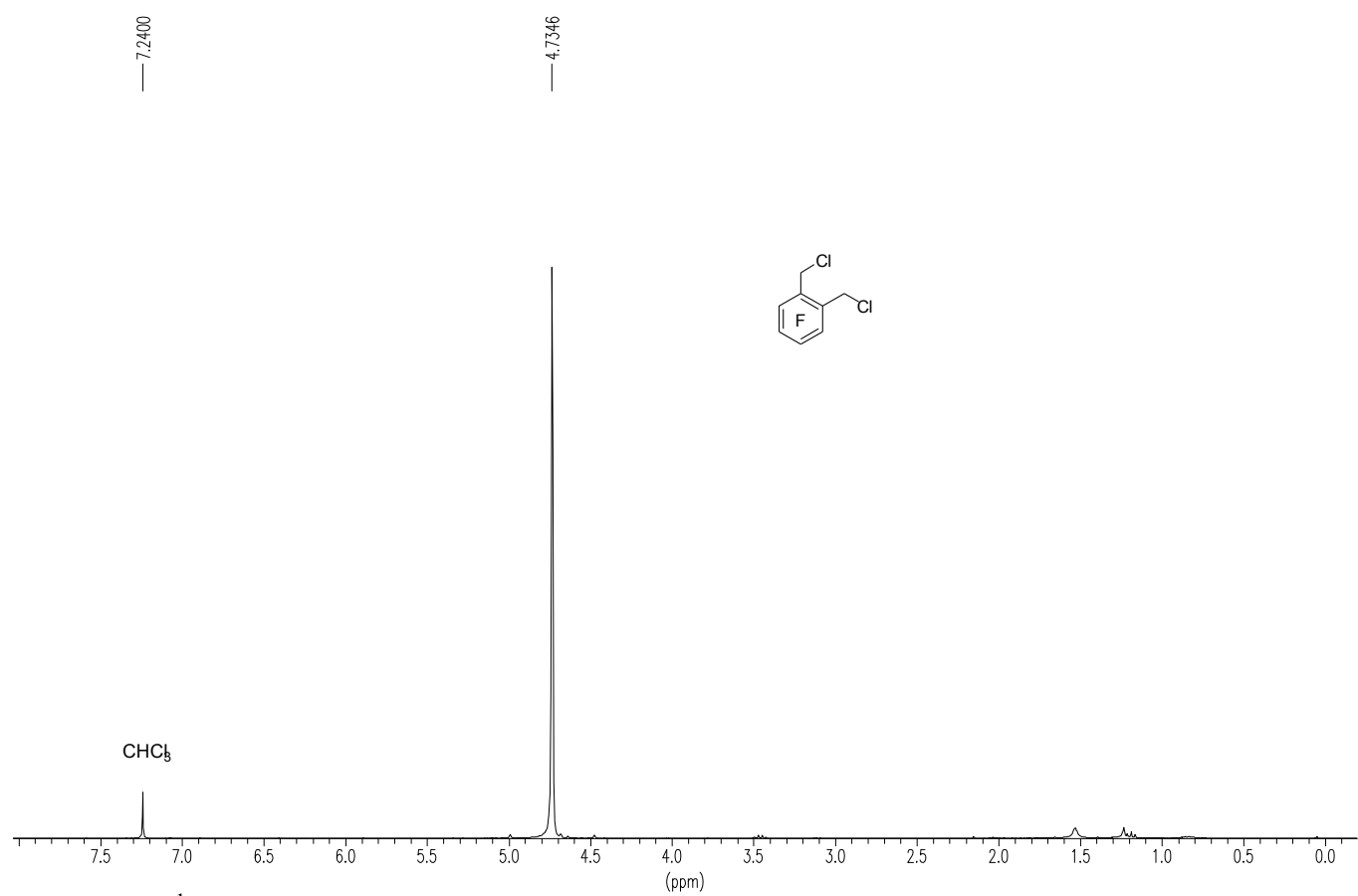


Figure S52. ¹H NMR spectrum of **16c** (CDCl₃).

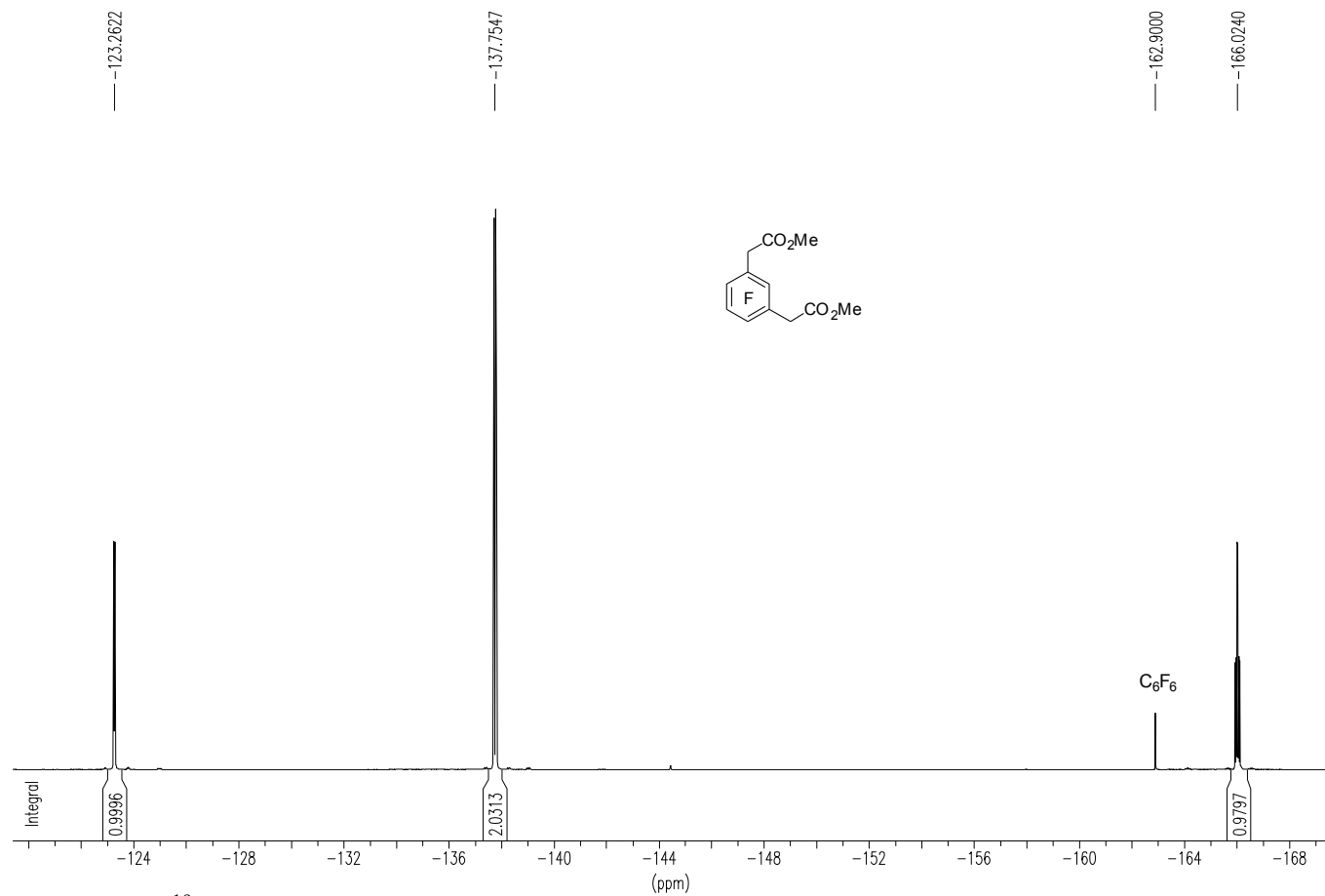


Figure S53. ^{19}F NMR spectrum of **17'b** (CDCl₃).

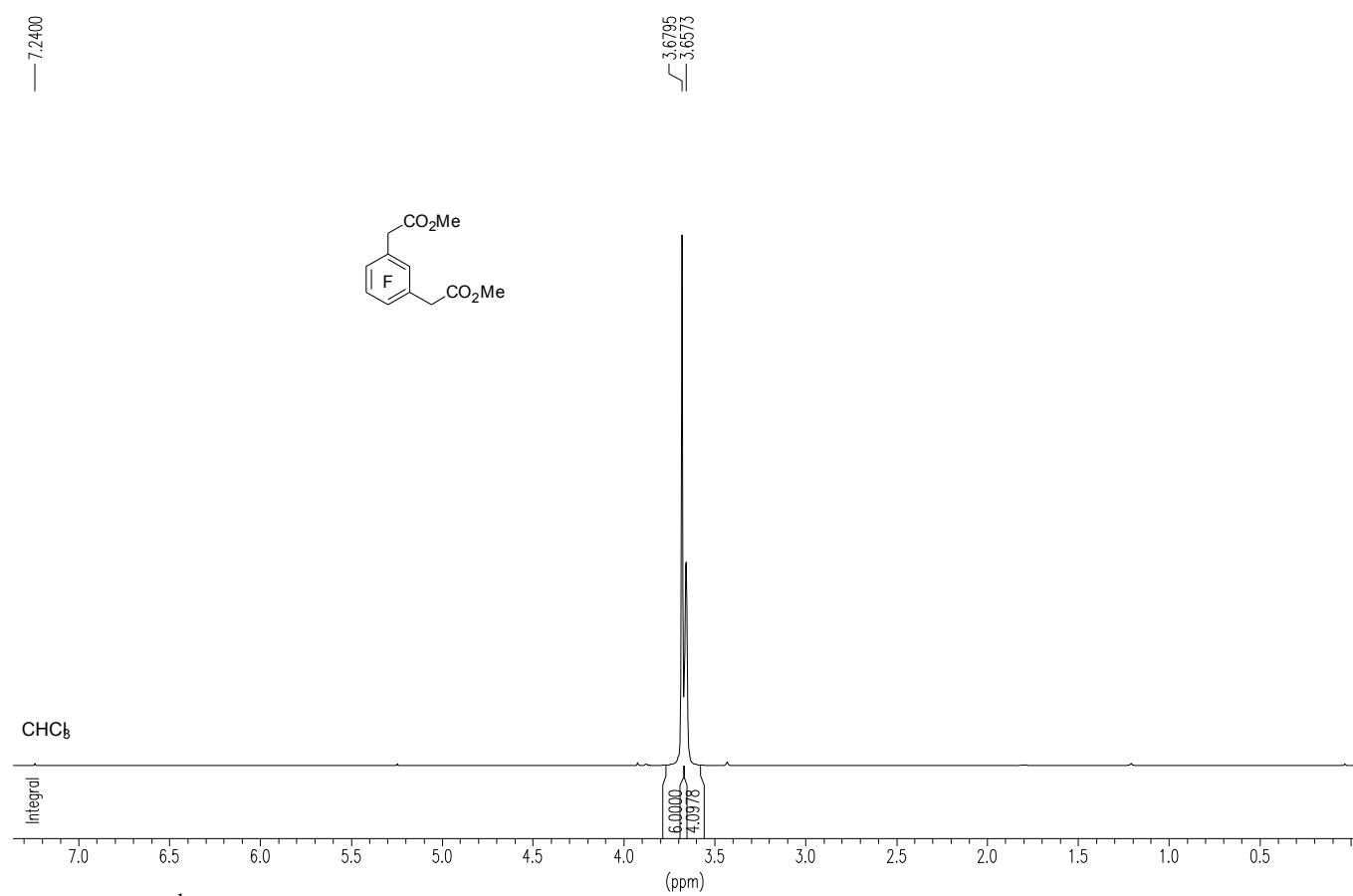


Figure S54. ^1H NMR spectrum of **17'b** (CDCl₃).

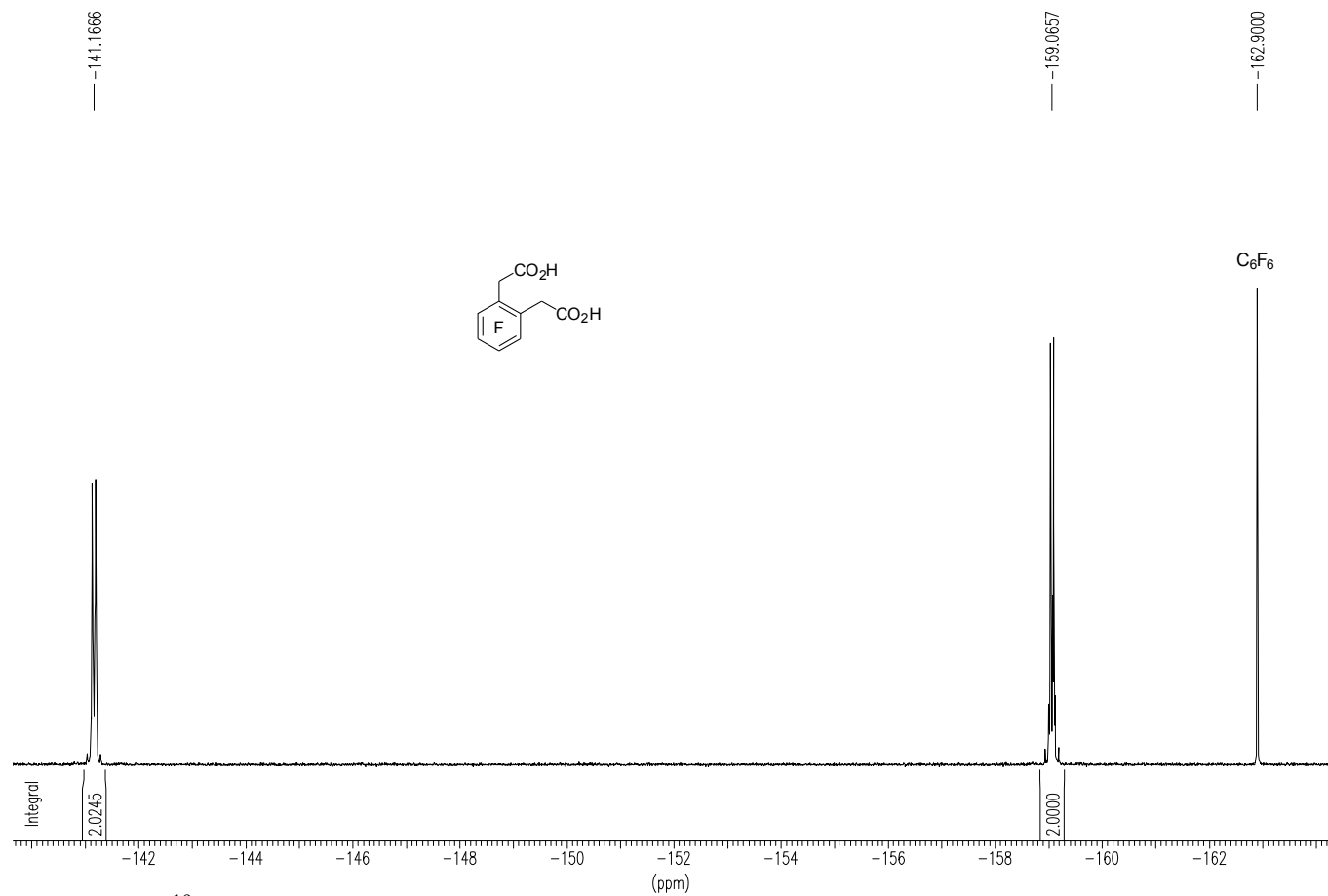


Figure S55. ¹⁹F NMR spectrum of **17c** (acetone-*d*₆).

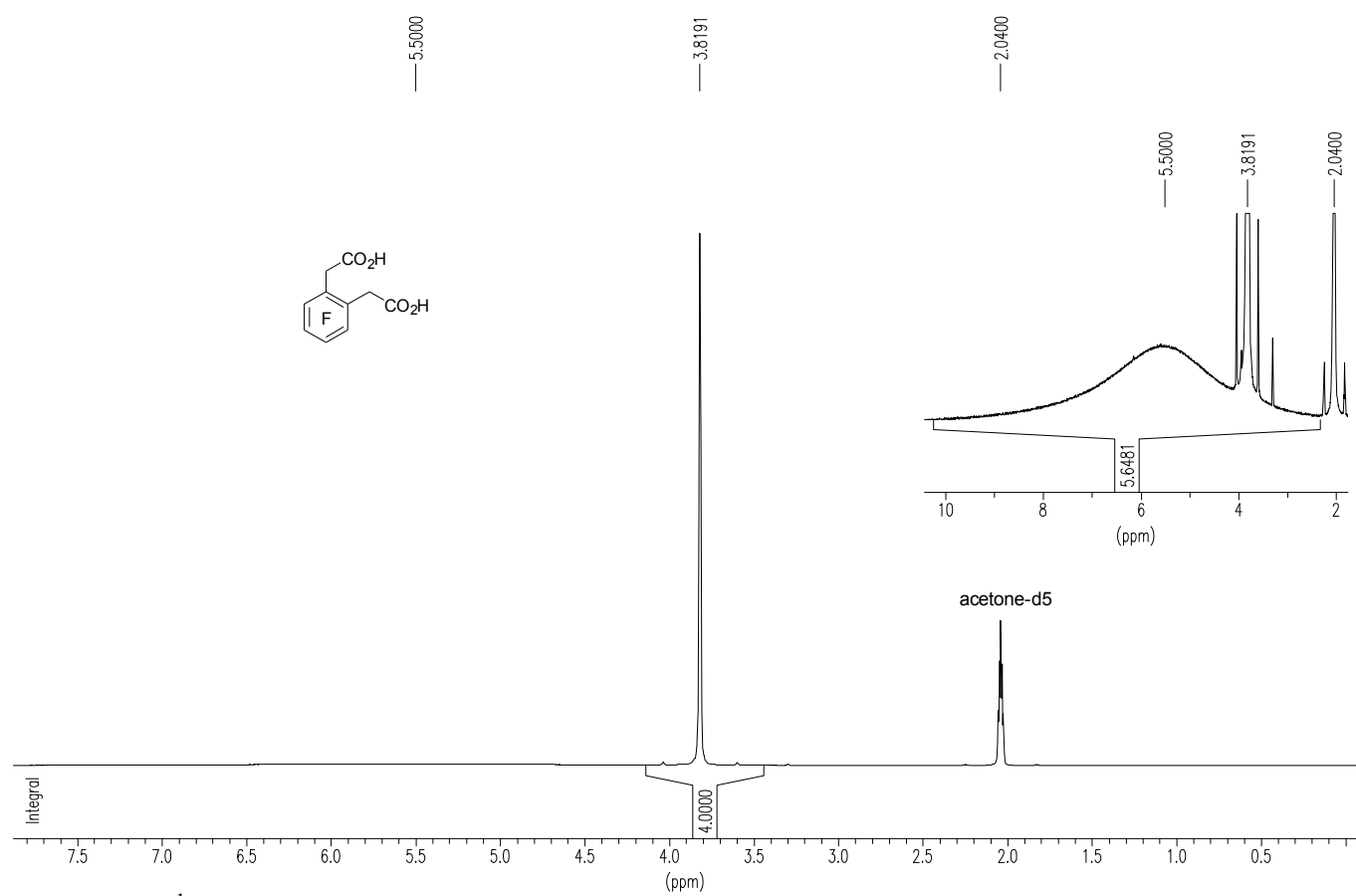


Figure S56. ¹H NMR spectrum of **17c** (acetone-*d*₆).

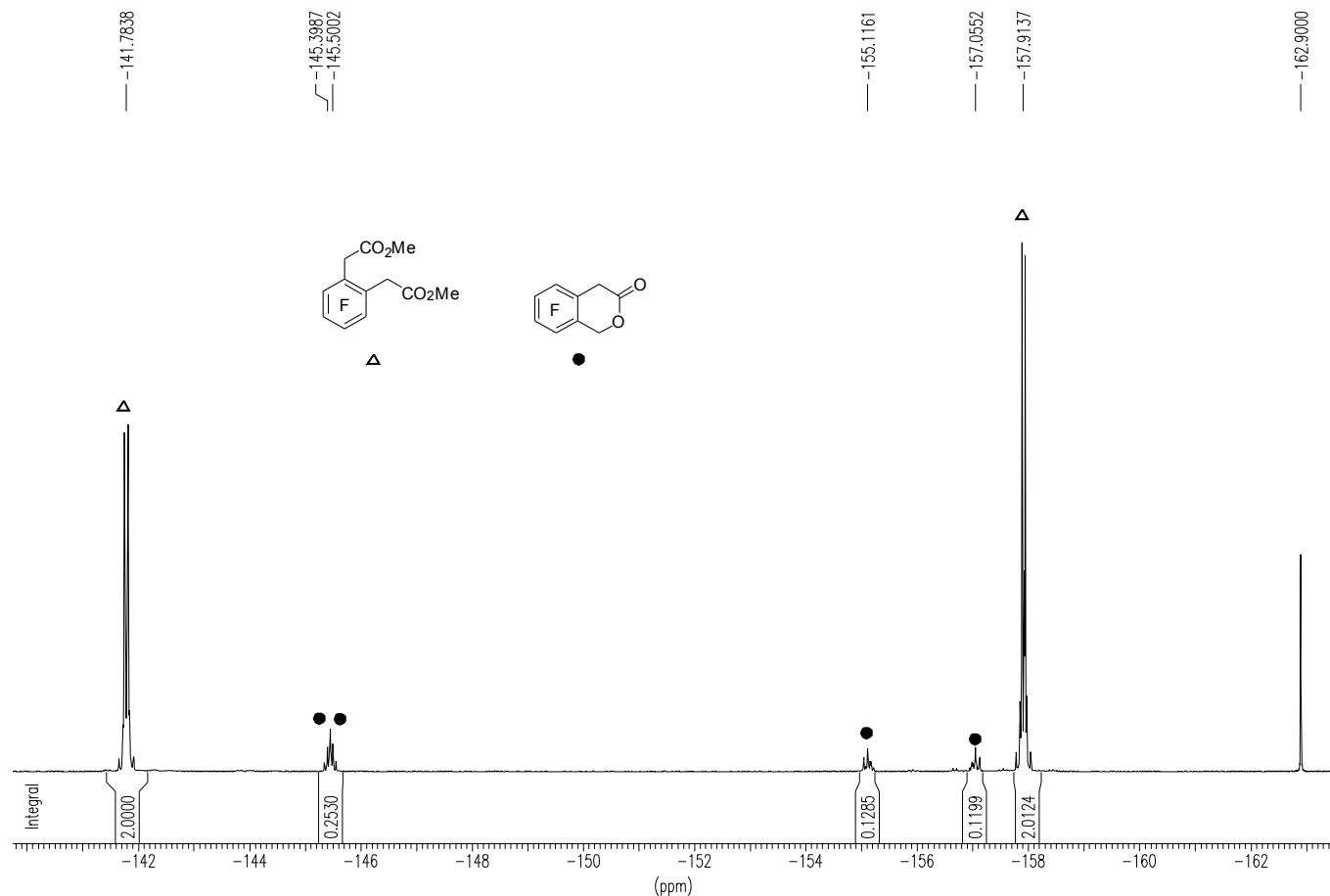


Figure S57. ¹⁹F NMR spectrum of a mixture of **17'c** and **15** (CDCl₃).

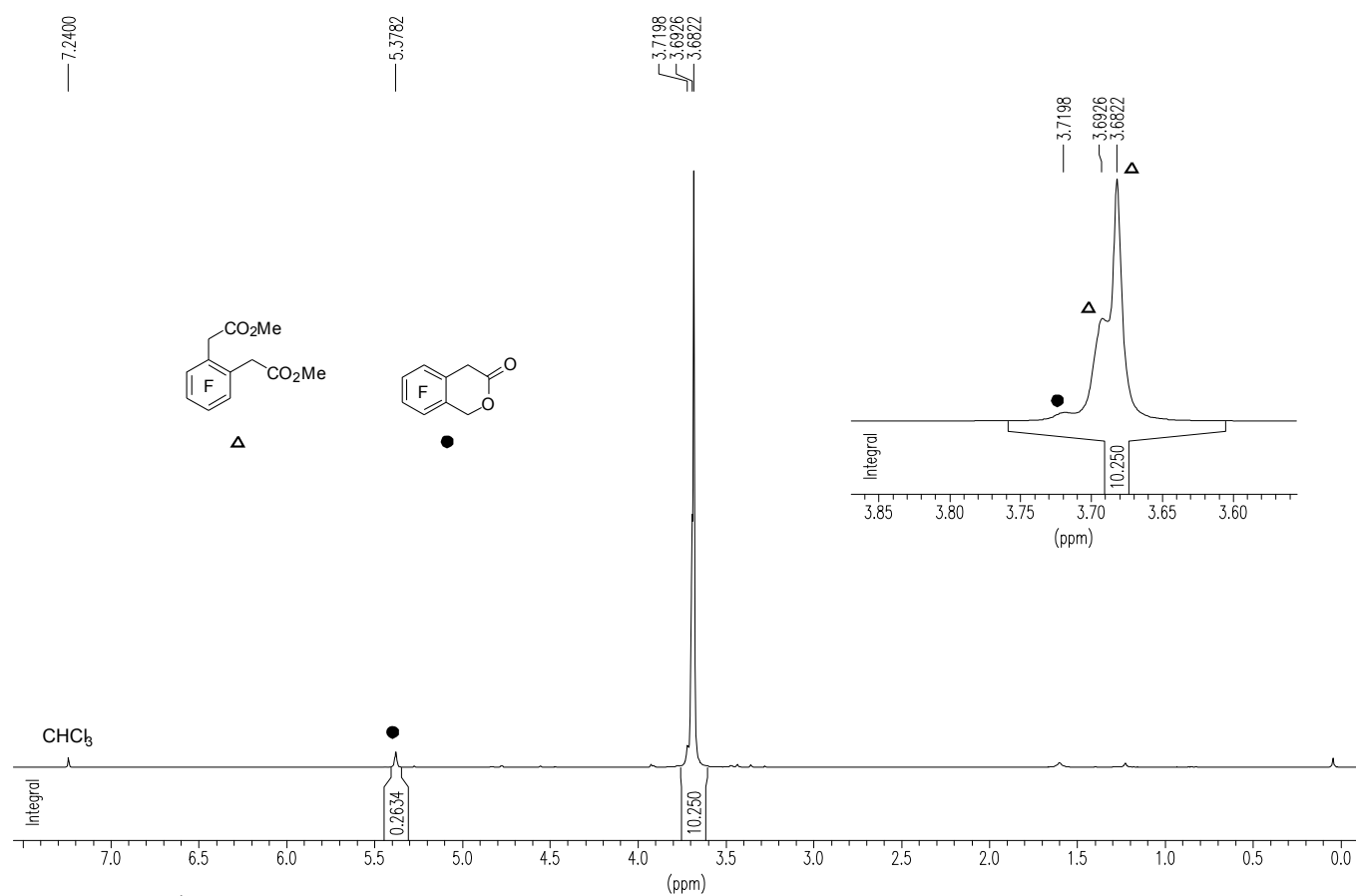


Figure S58. ¹H NMR spectrum of a mixture of **17'c** and **15** (CDCl₃).

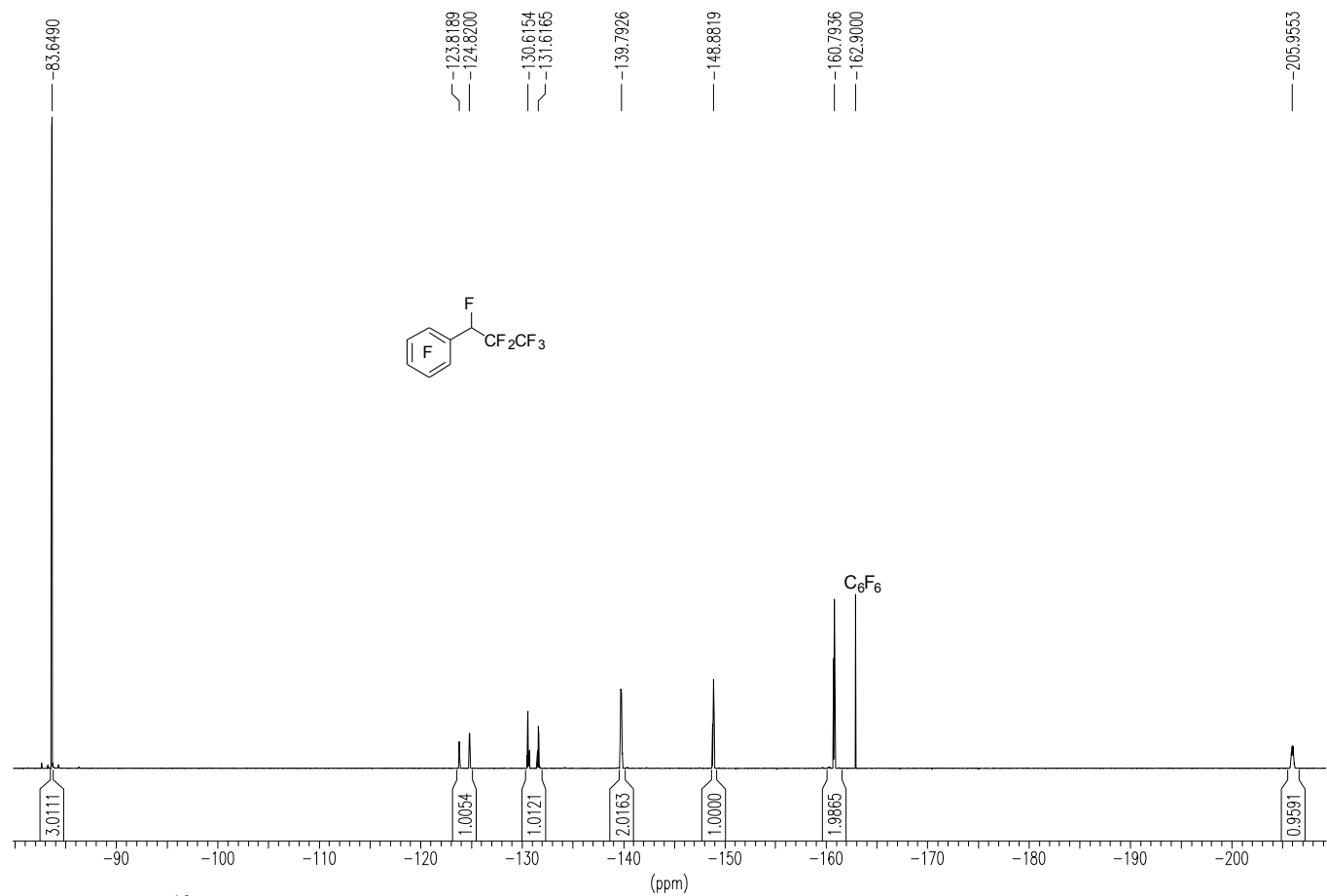


Figure S59. ^{19}F NMR spectrum of **22b** (CDCl_3).

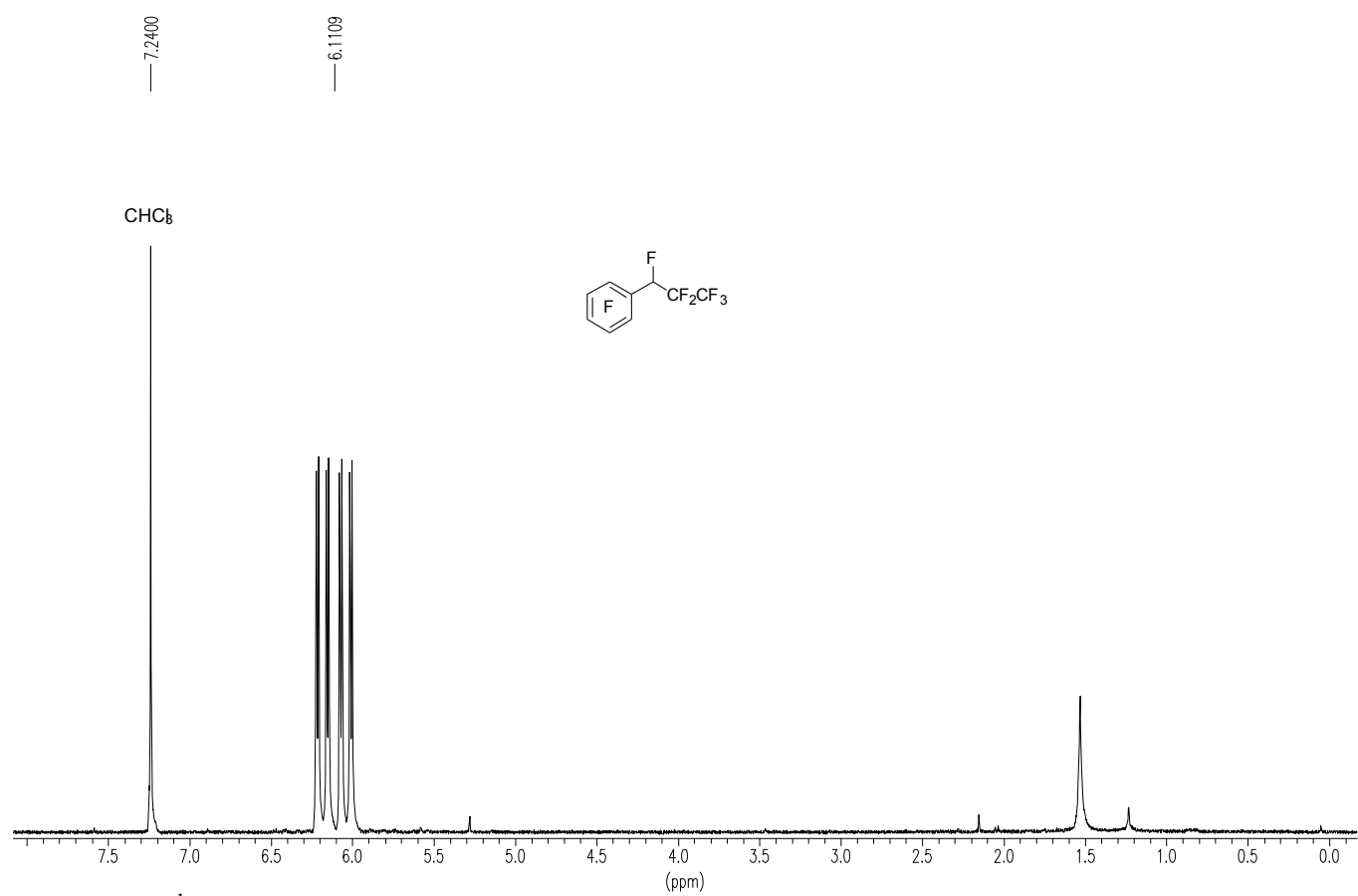


Figure S60. ^1H NMR spectrum of **22b** (CDCl_3).

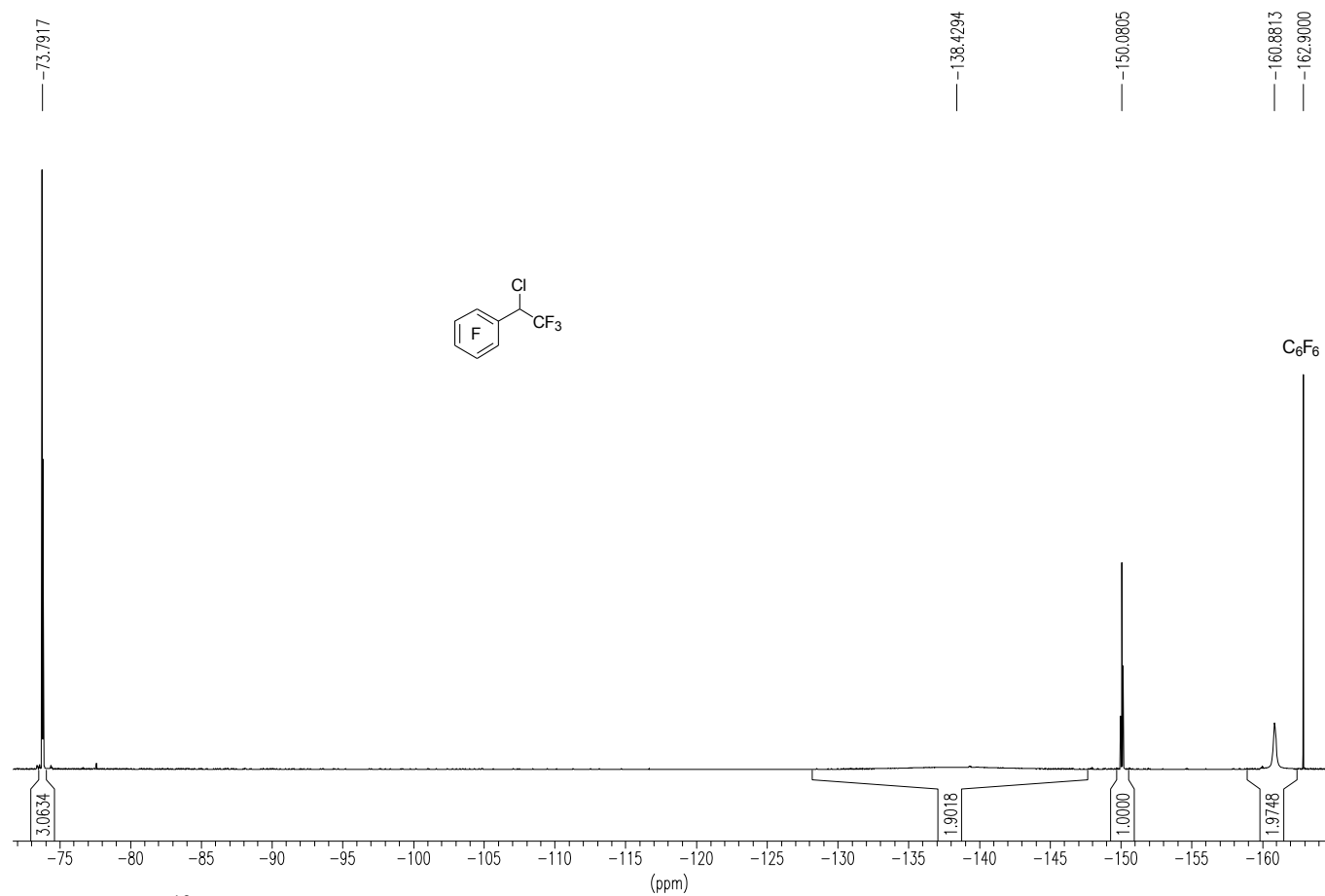


Figure S61. ¹⁹F NMR spectrum of **23a** (CDCl₃).

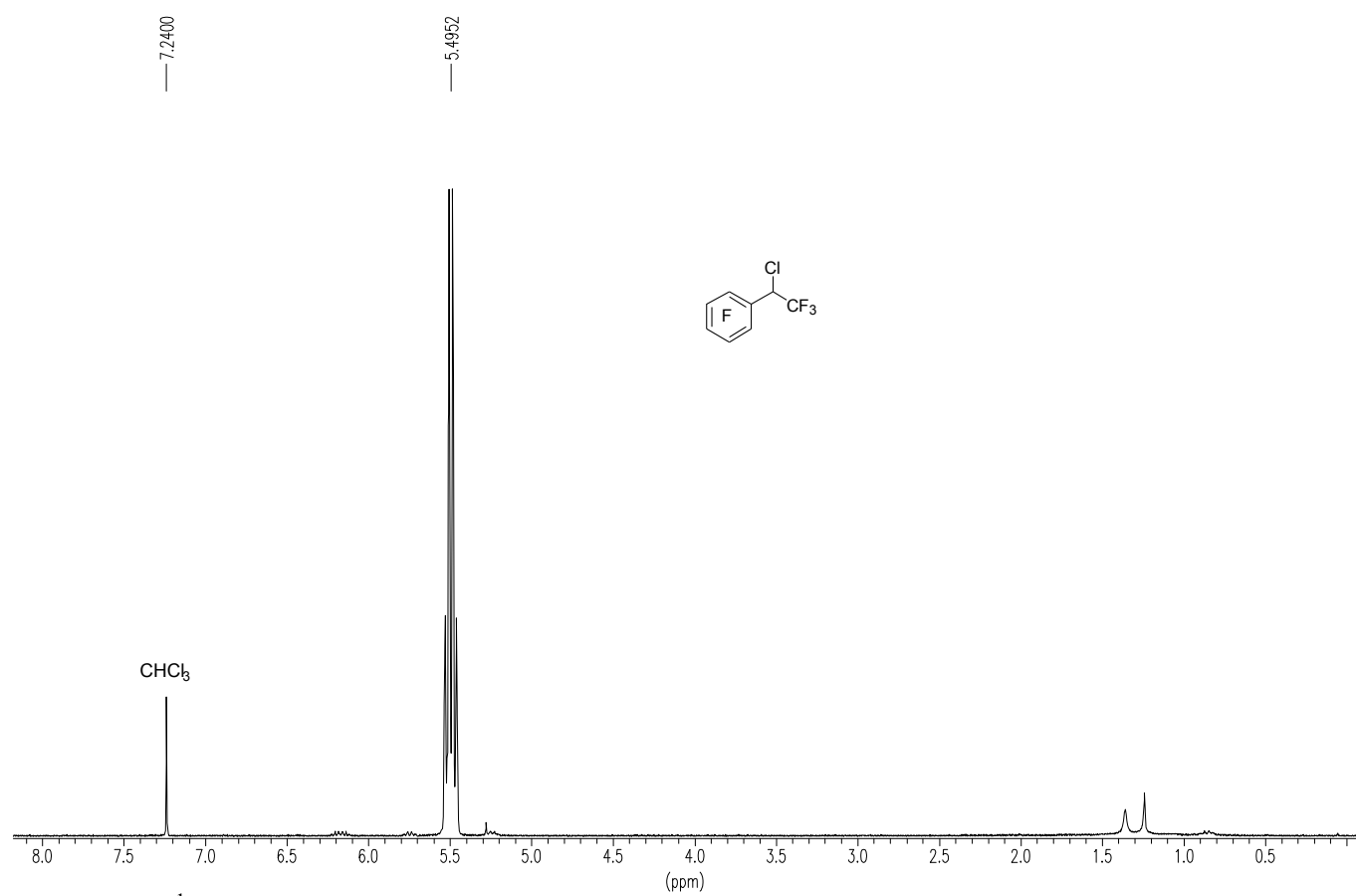


Figure S62. ¹H NMR spectrum of **23a** (CDCl₃).

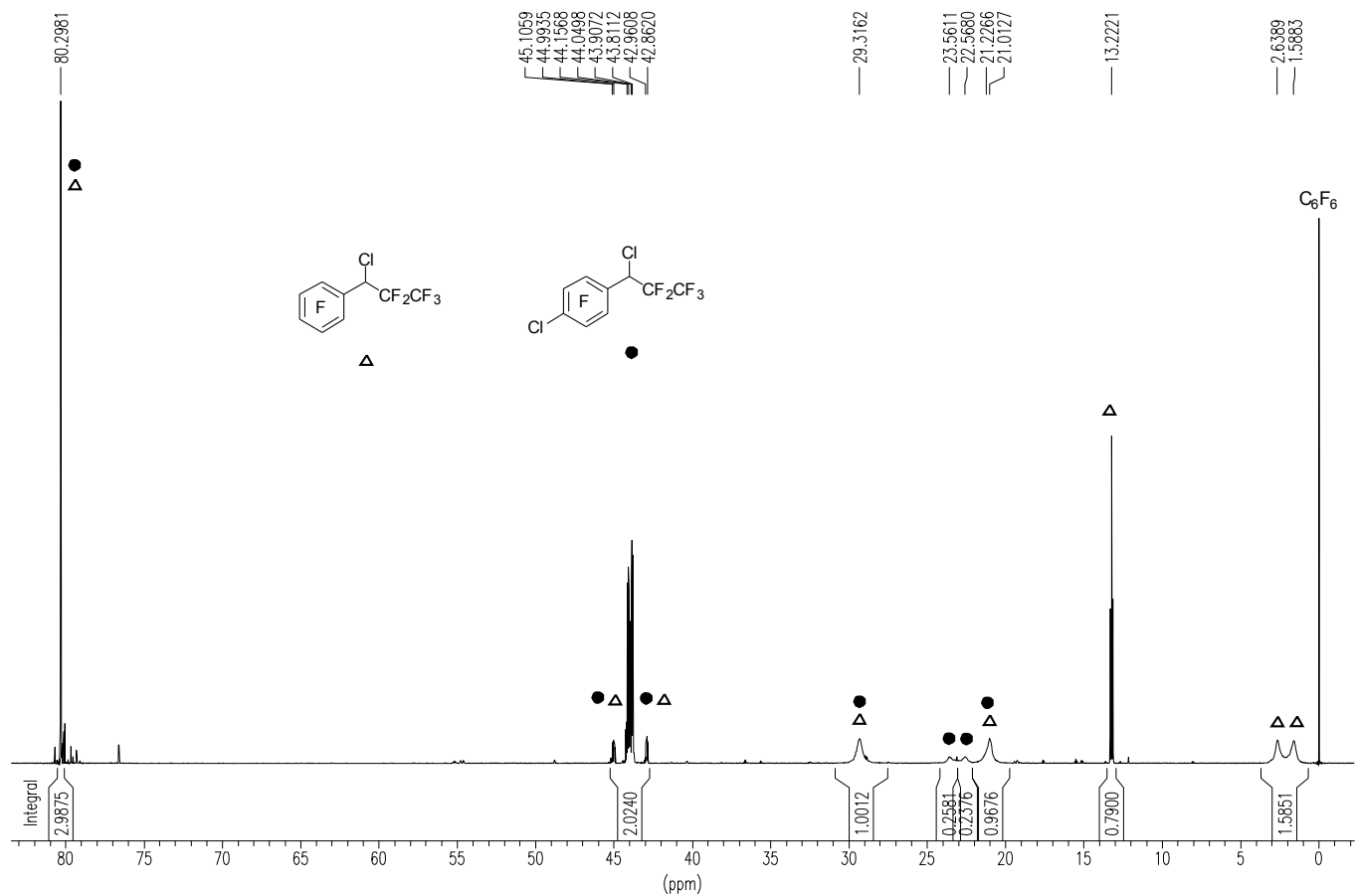


Figure S63. ^{19}F NMR spectrum of a mixture of **23b** and **45** (CDCl_3).

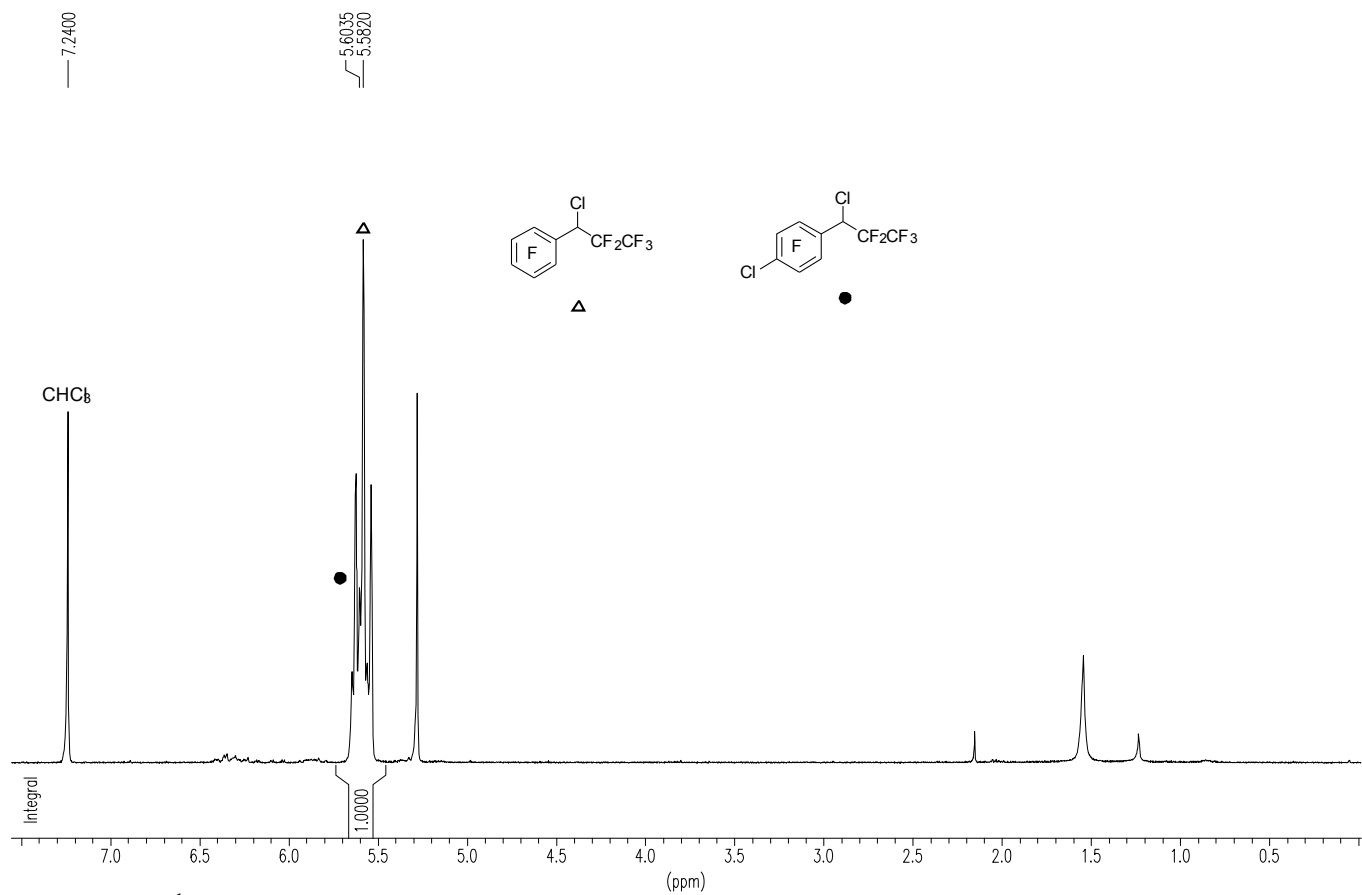


Figure S64. ^1H NMR spectrum of a mixture of **23b** and **45** (CDCl_3).

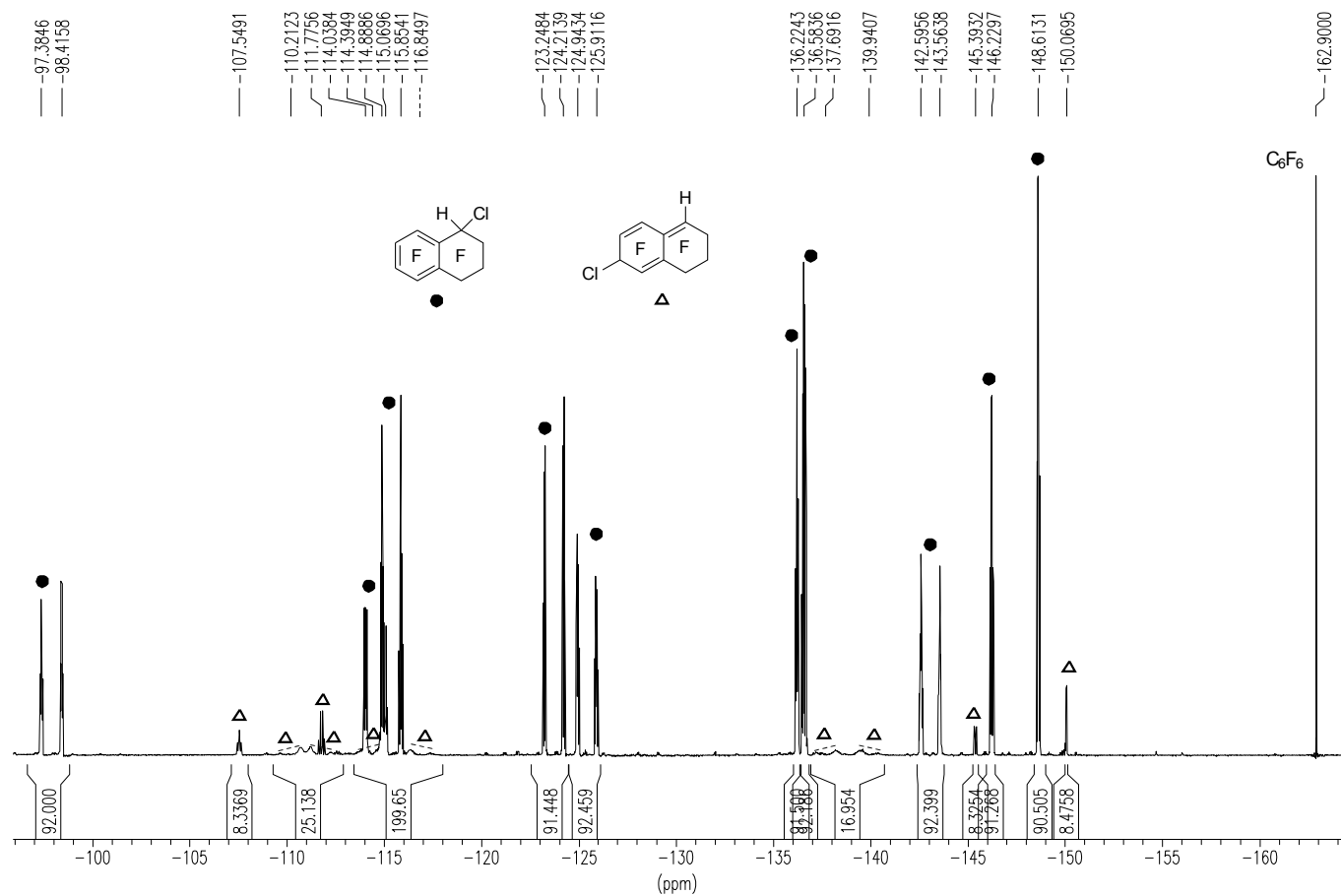


Figure S65. ^{19}F NMR spectrum of a mixture of **23c** and **47** (CDCl_3).

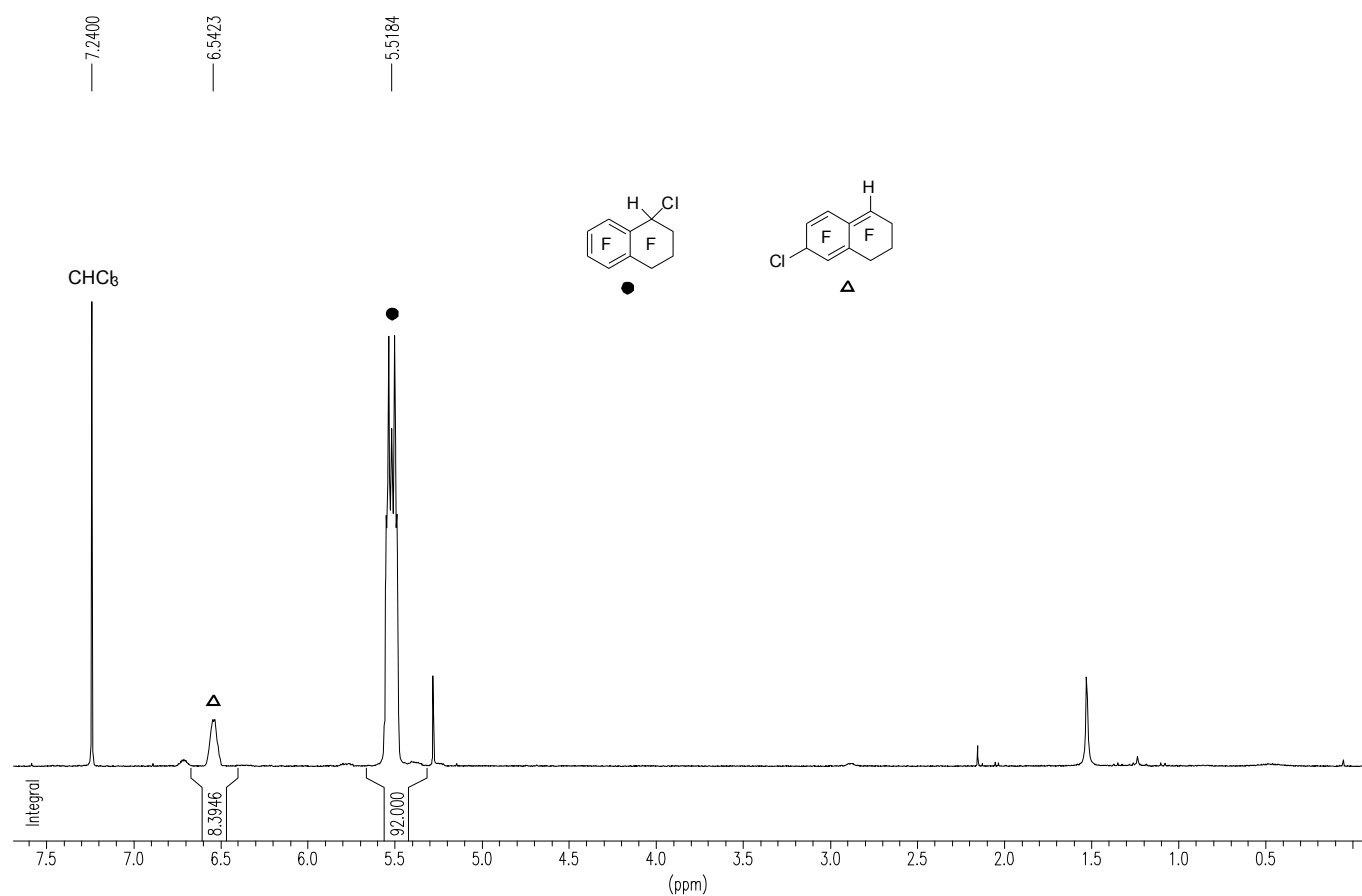


Figure S66. ^1H NMR spectrum of a mixture of **23c** and **47** (CDCl_3).

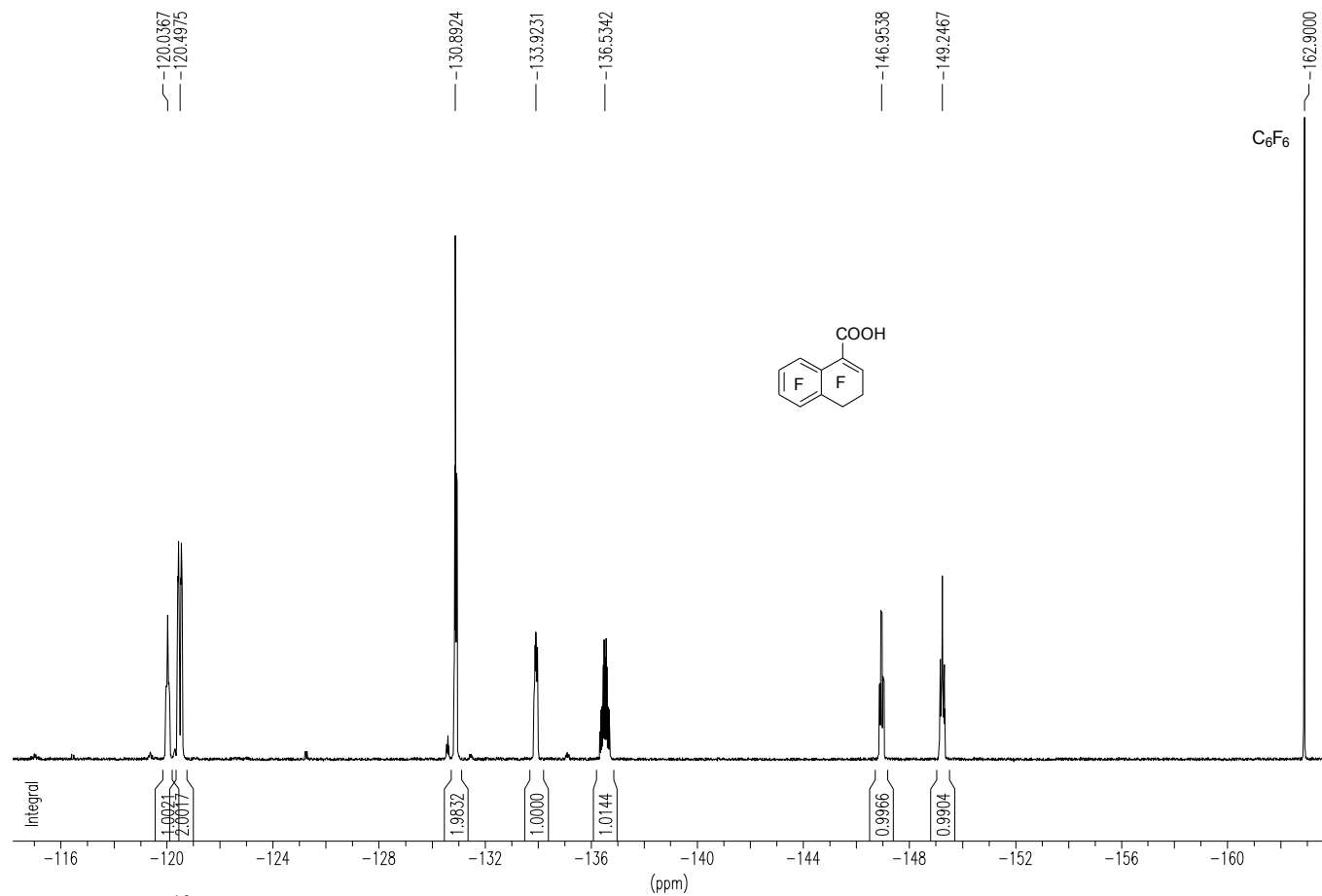


Figure S67. ¹⁹F NMR spectrum of **25c** (CDCl₃).

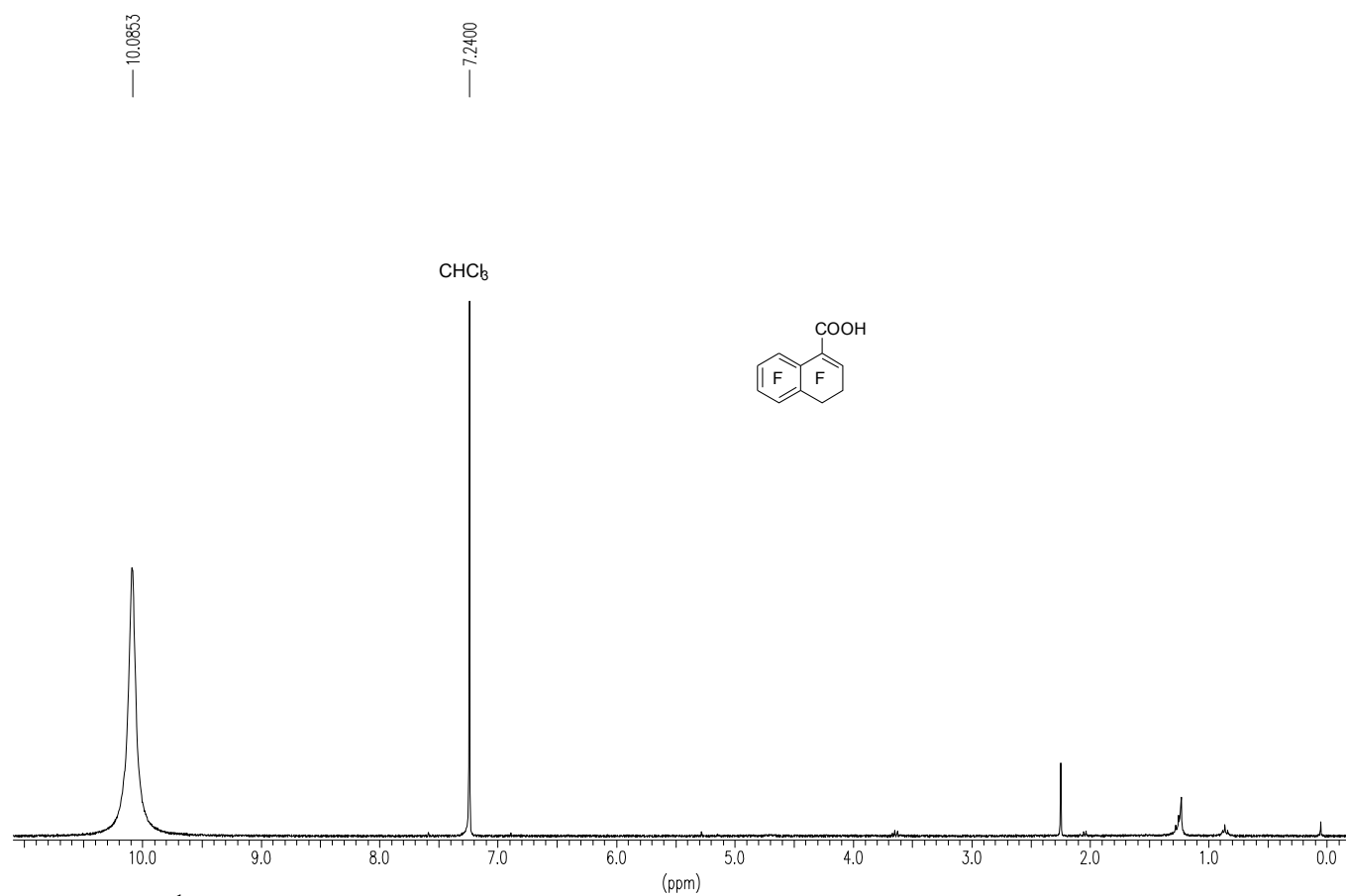


Figure S68. ¹H NMR spectrum of **25c** (CDCl₃).

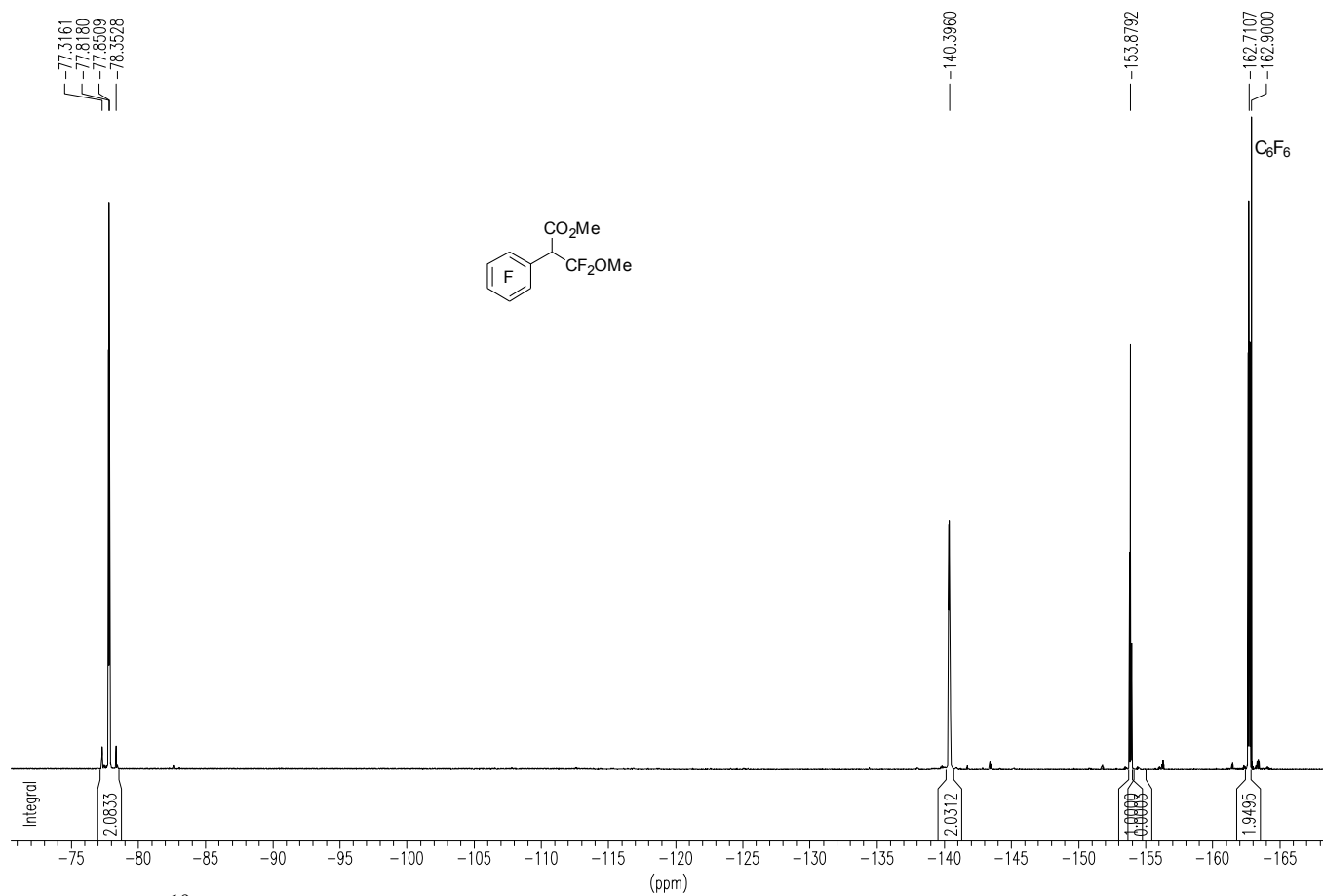


Figure S69. ¹⁹F NMR spectrum of **28'** (CDCl₃).

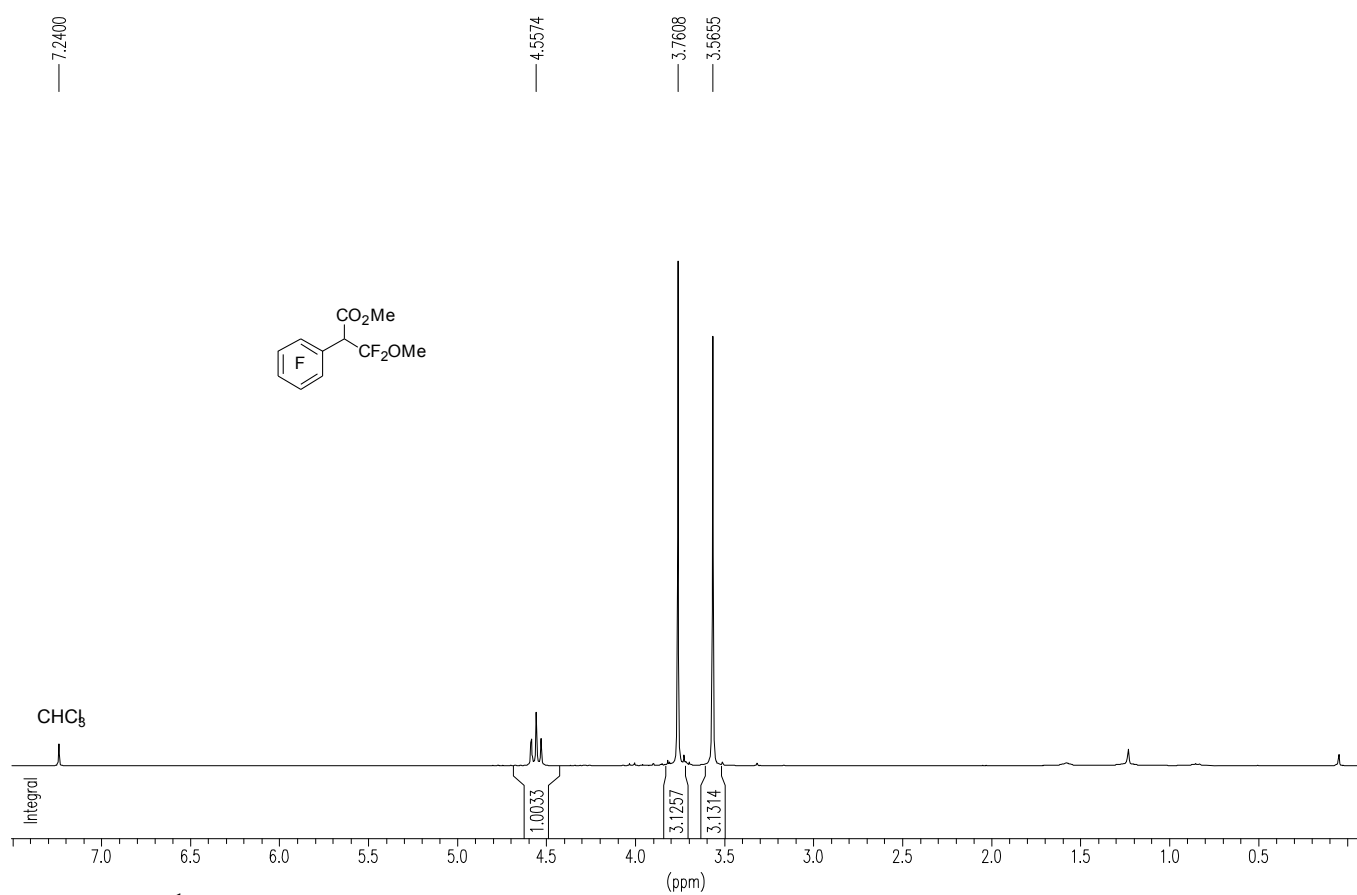


Figure S70. ¹H NMR spectrum of **28'** (CDCl₃).

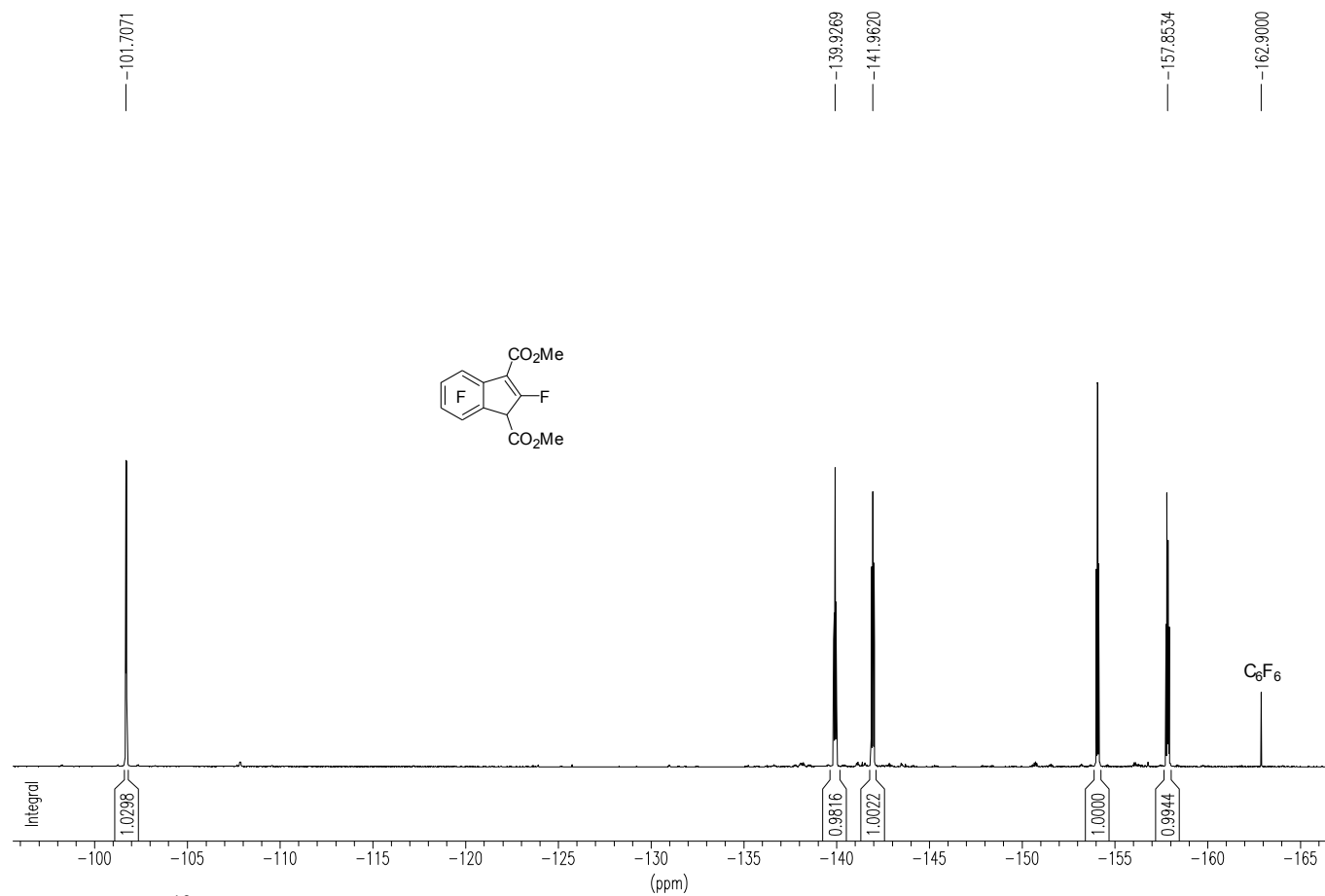


Figure S71. ¹⁹F NMR spectrum of **29'** (CDCl₃).

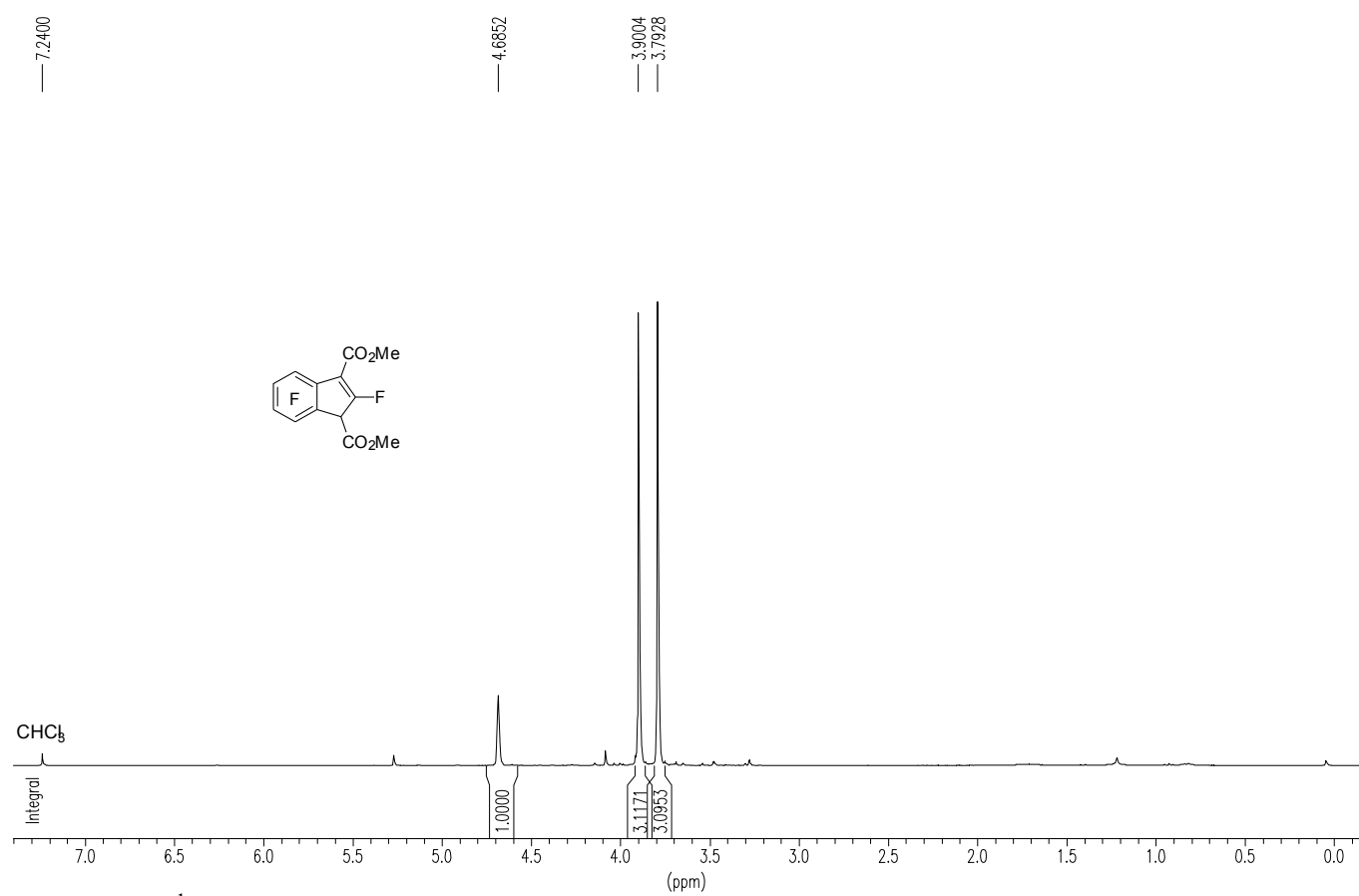


Figure S72. ¹H NMR spectrum of **29'** (CDCl₃).

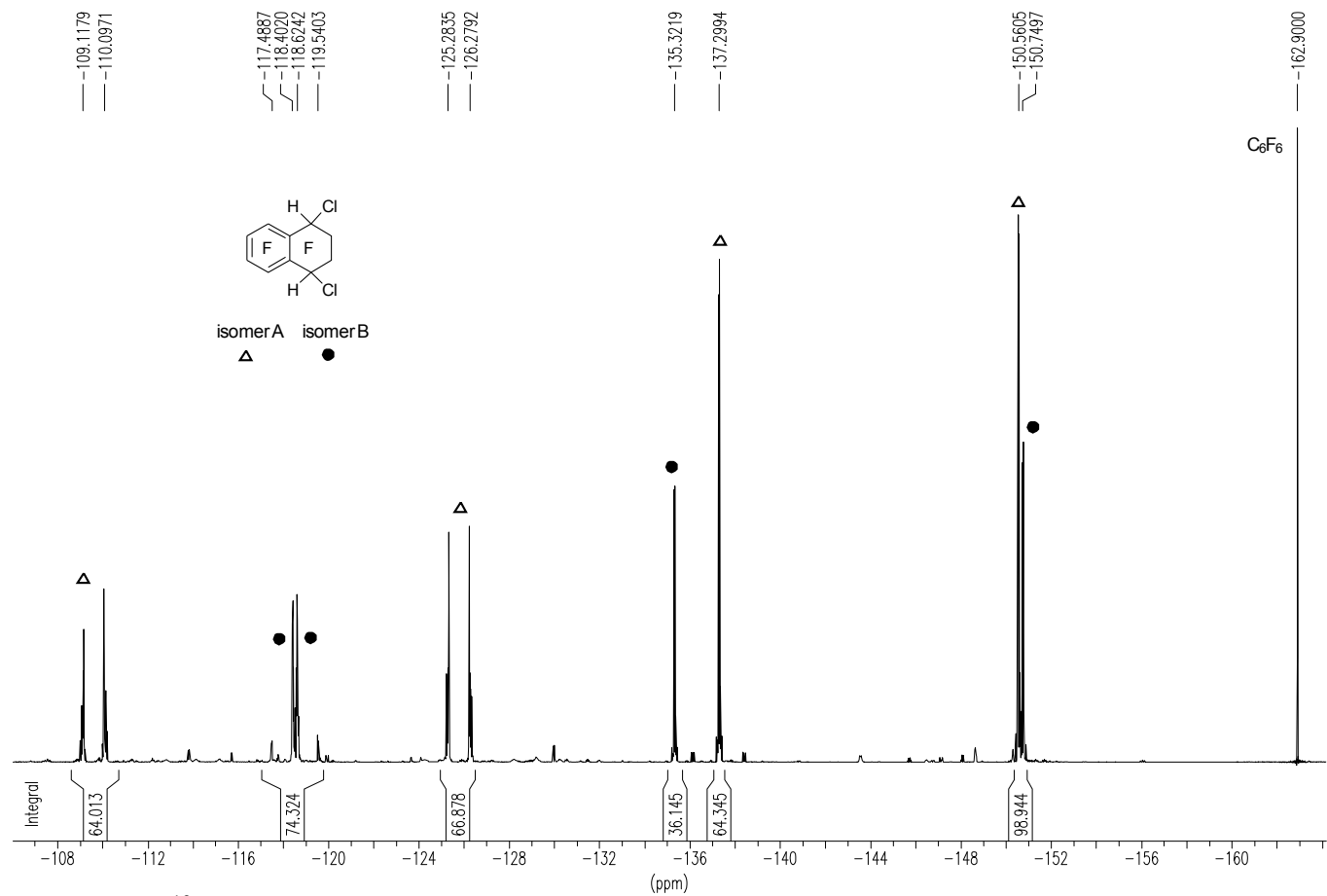


Figure S73. ¹⁹F NMR spectrum of **36** (CDCl₃).

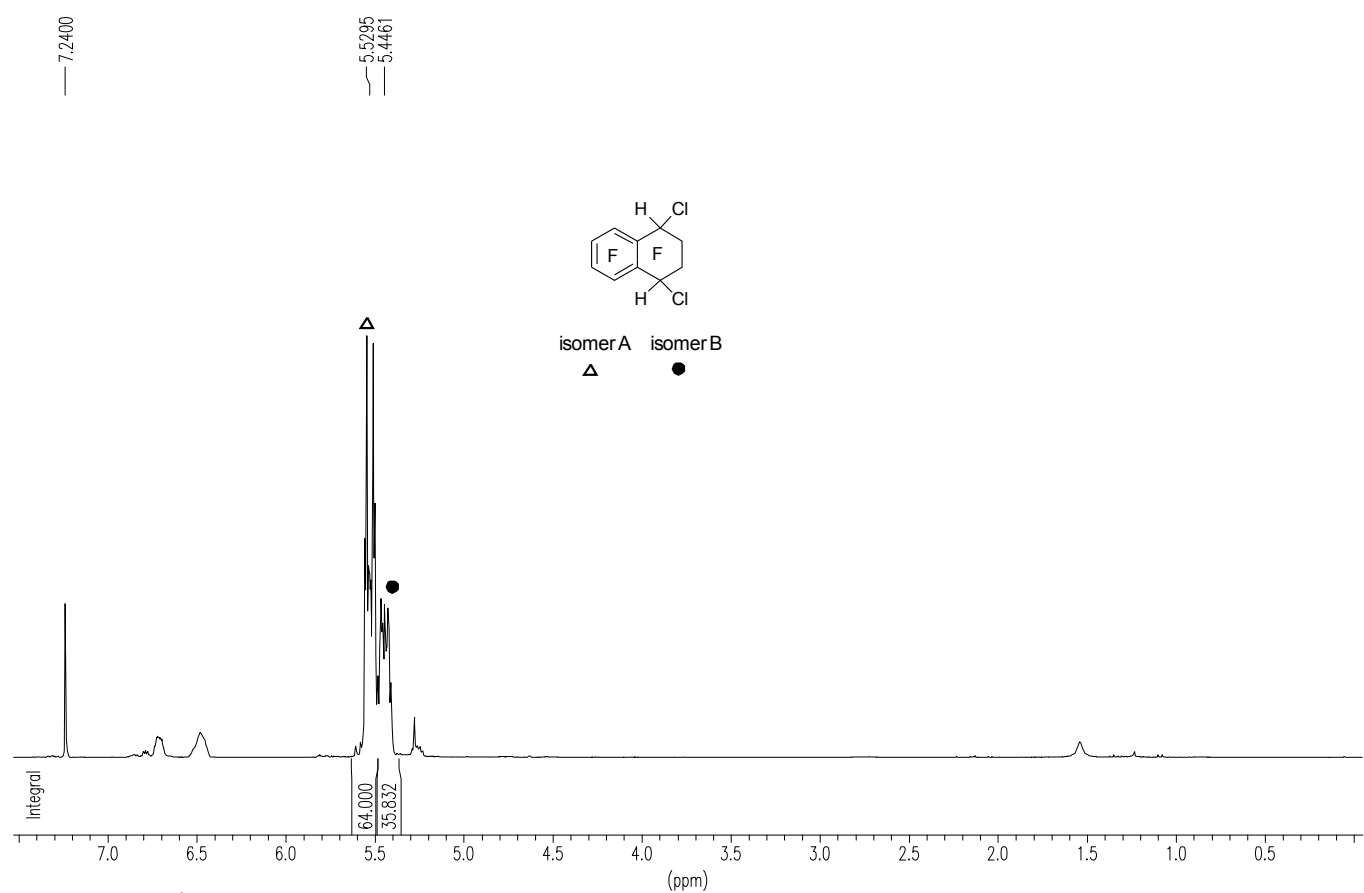


Figure S74. ¹H NMR spectrum of **36** (CDCl₃).

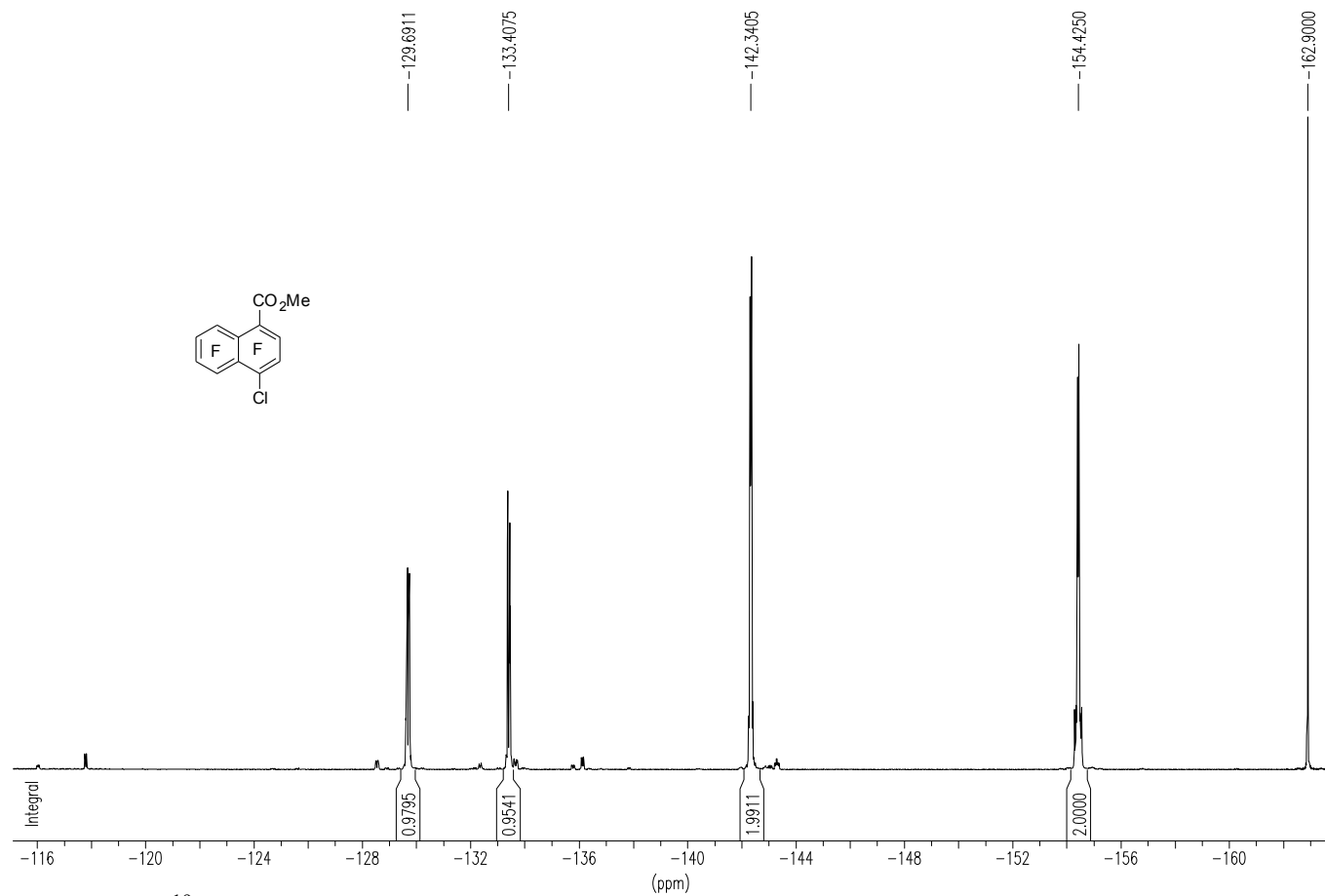


Figure S75. ¹⁹F NMR spectrum of **38'** (CDCl₃).

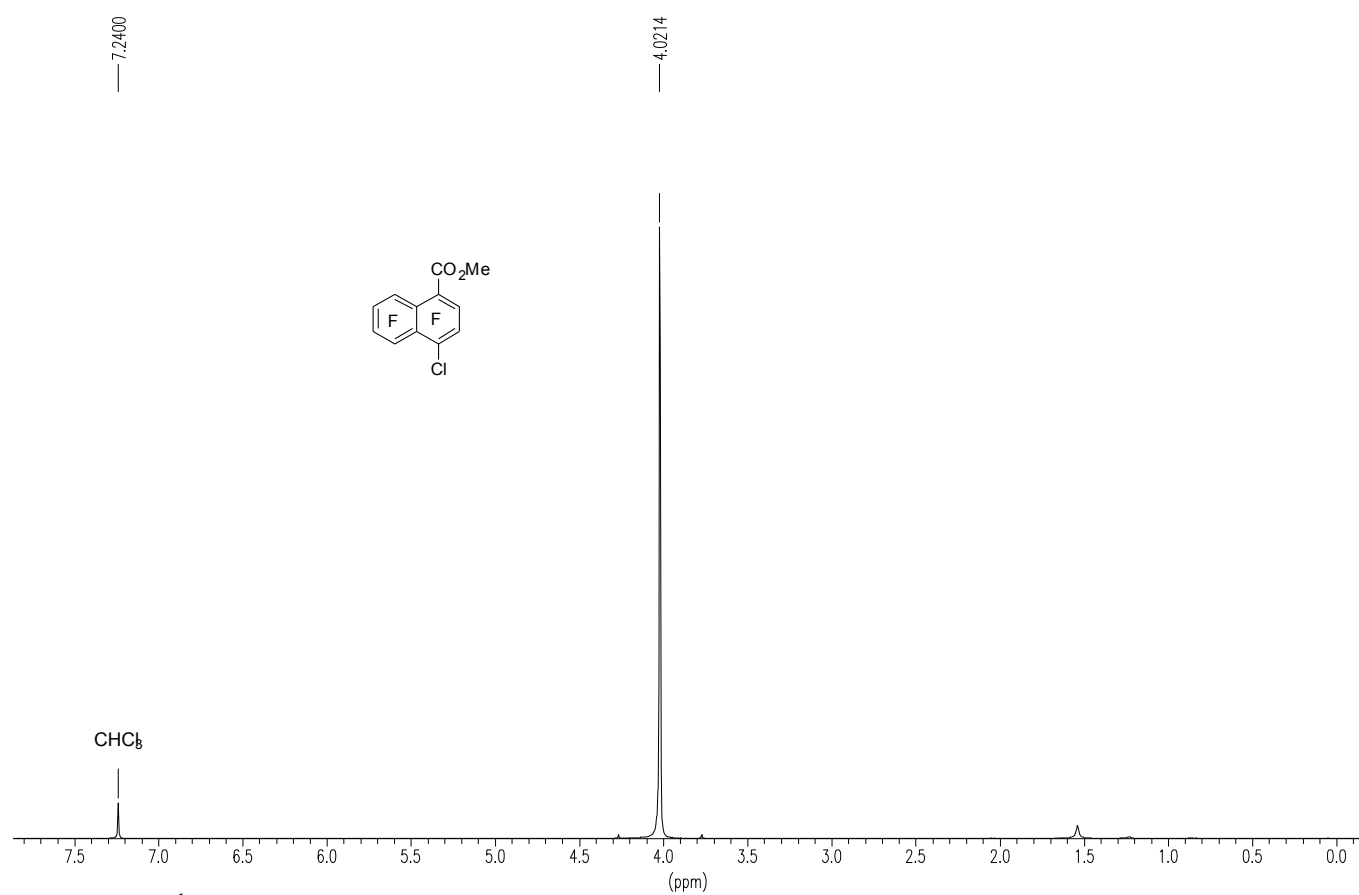
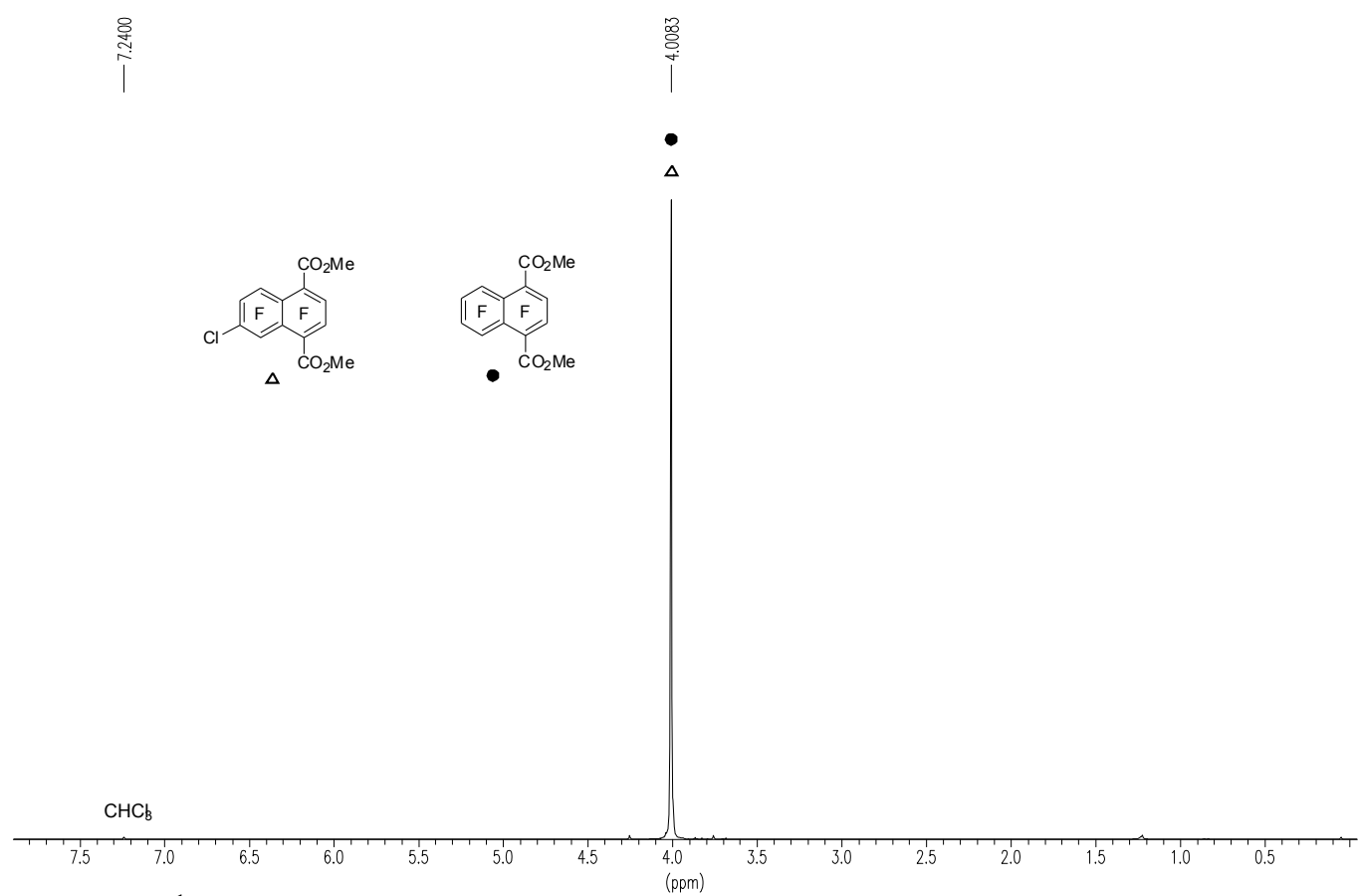
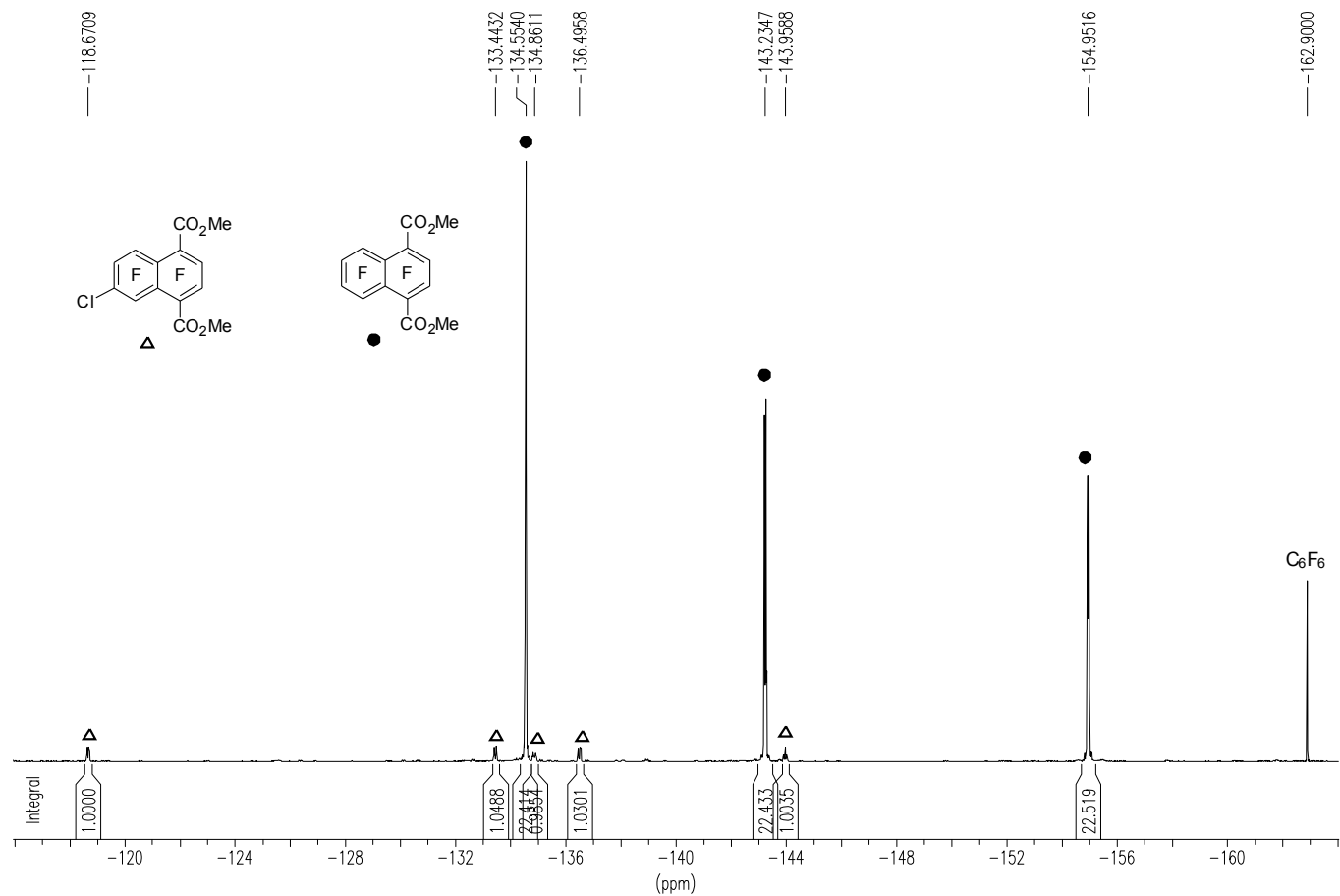


Figure S76. ¹H NMR spectrum of **38'** (CDCl₃).



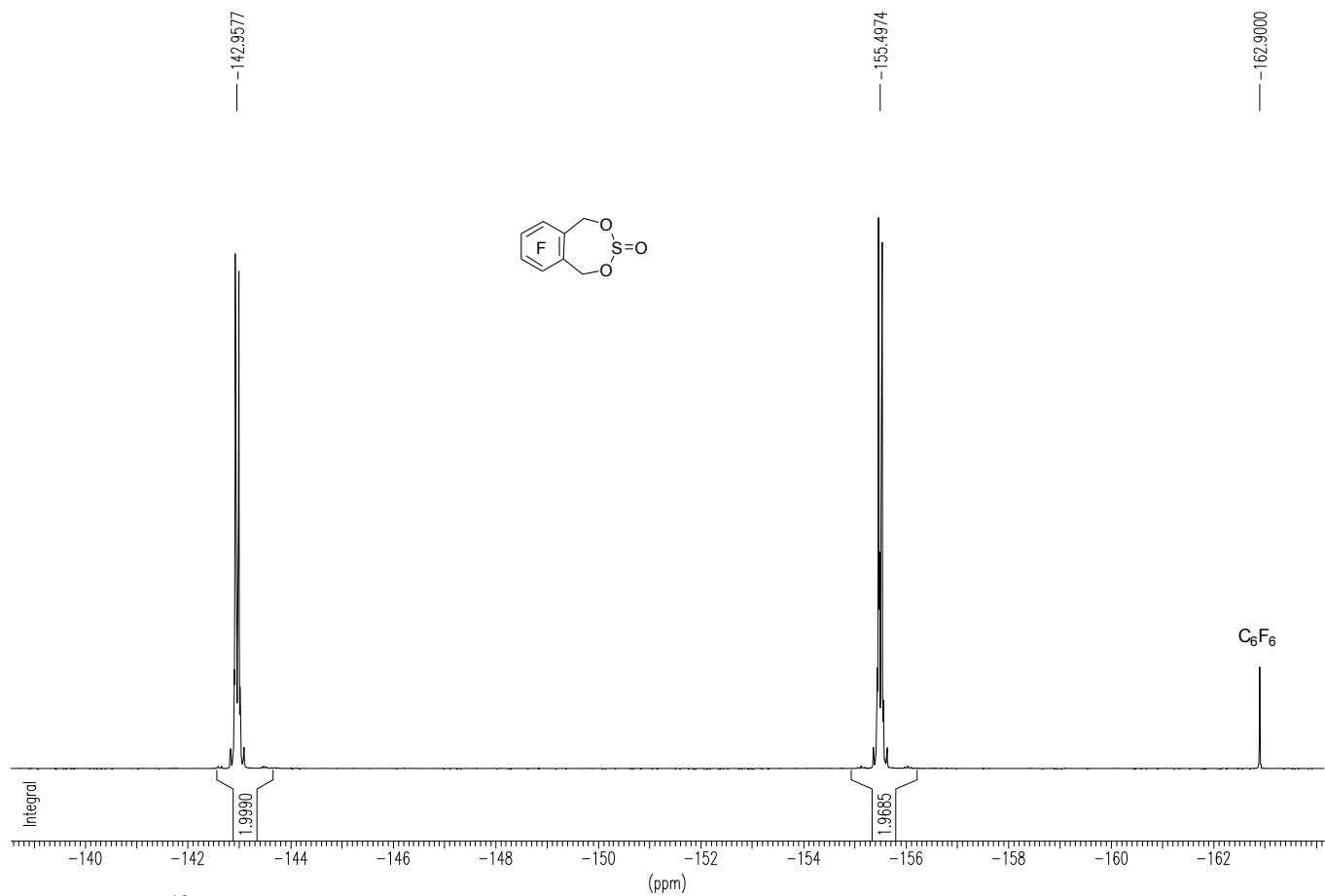


Figure S79. ¹⁹F NMR spectrum of **44** (CDCl₃).

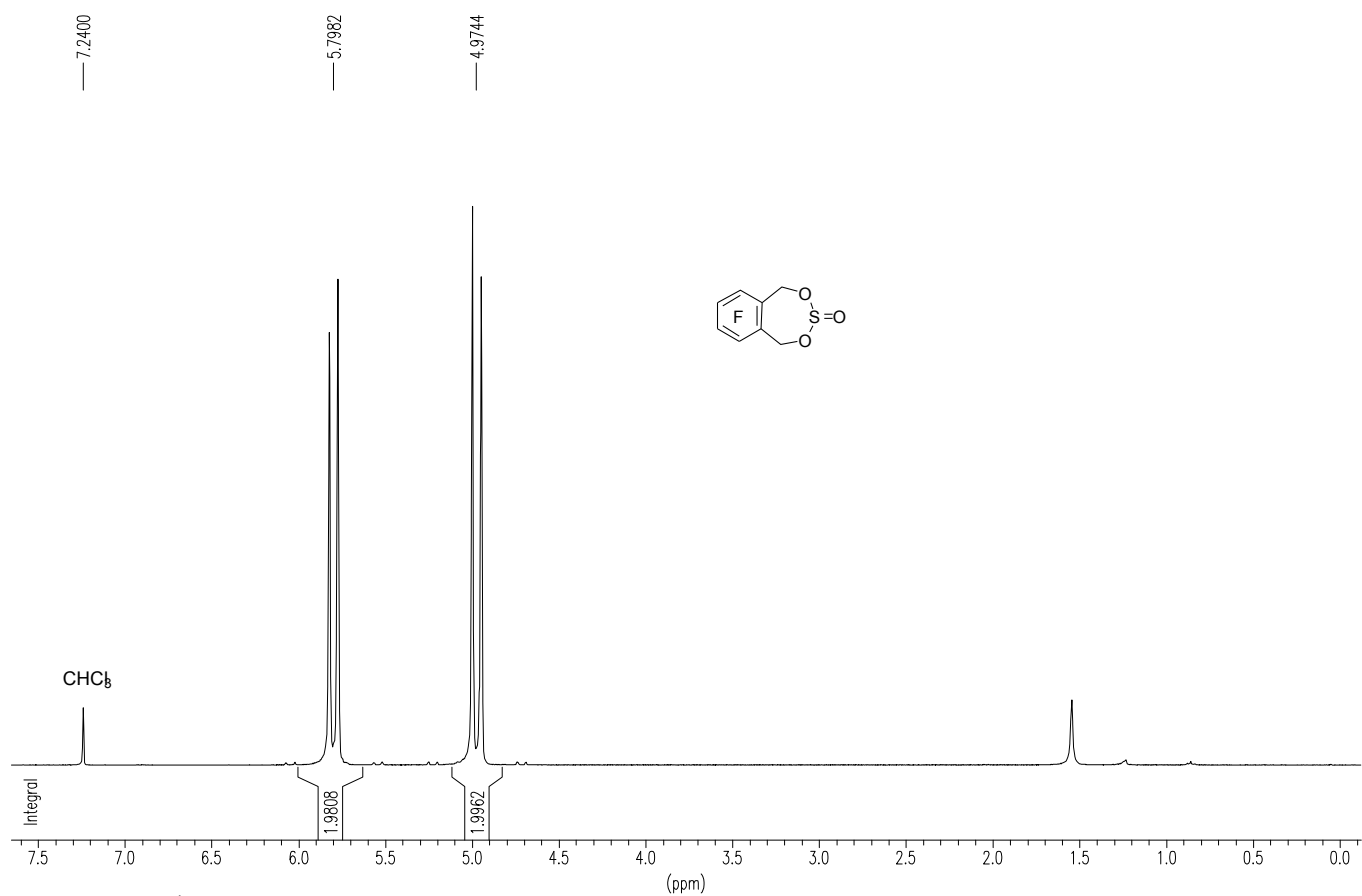


Figure S80. ¹H NMR spectrum of **44** (CDCl₃).