

Supporting Information

F-THENA: A Chiral Derivatizing Agent for the Determination of the Absolute Configuration of Secondary Aromatic Alcohols with Self-Validating System

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^1H NMR and ^{13}C NMR spectra

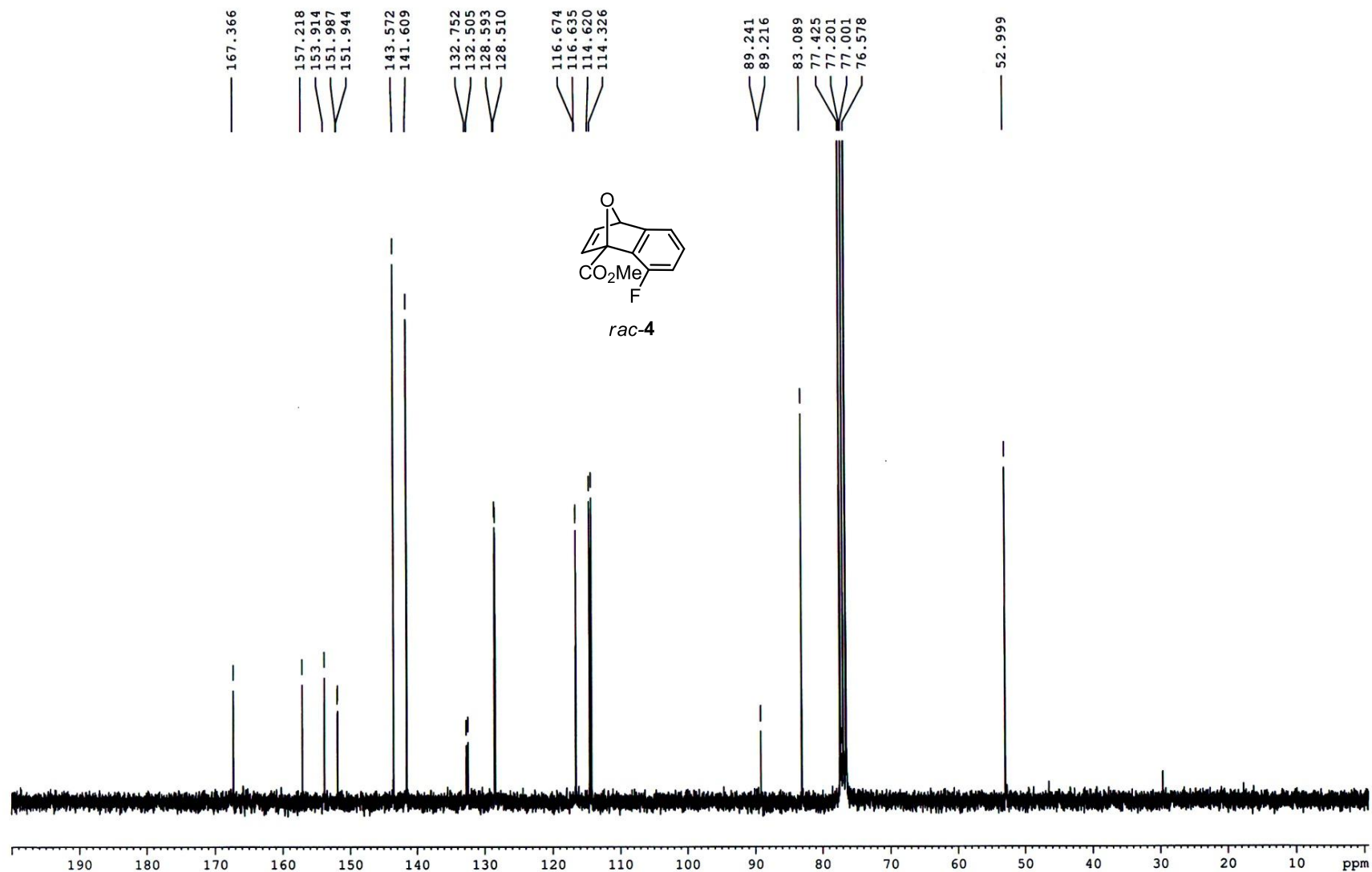


Figure 2. ^{13}C NMR spectrum of methyl 8-fluoro-1,4-dihydro-1,4-epoxynaphthalene-1-carboxylate (*rac-4*).

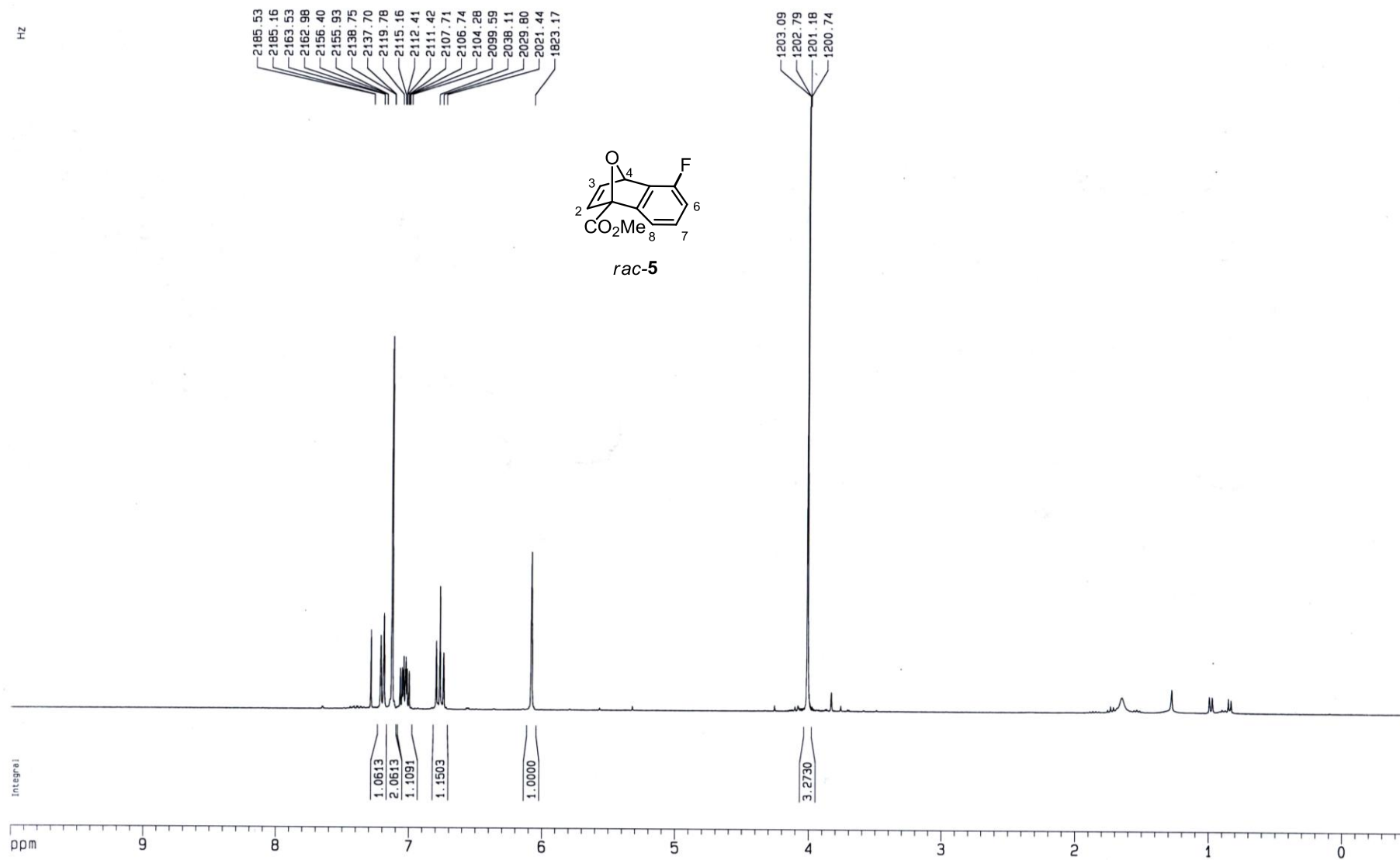


Figure 3. ¹H NMR spectrum of methyl 5-fluoro-1,4-dihydro-1,4-epoxynaphthalene-1-carboxylate (*rac*-5).

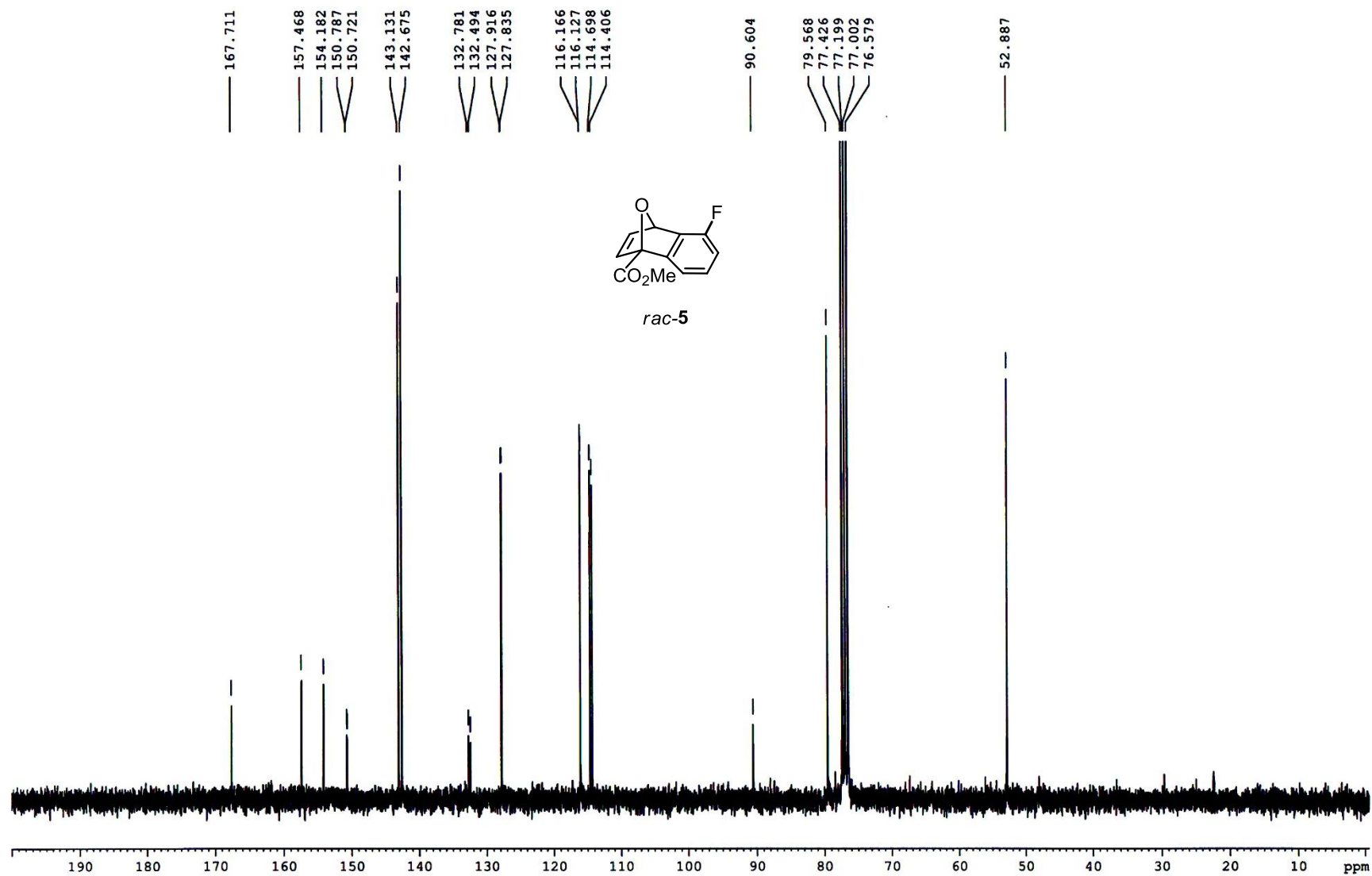


Figure 4. ^{13}C NMR spectrum of methyl 5-fluoro-1,4-dihydro-1,4-epoxynaphthalene-1-carboxylate (*rac*-5).

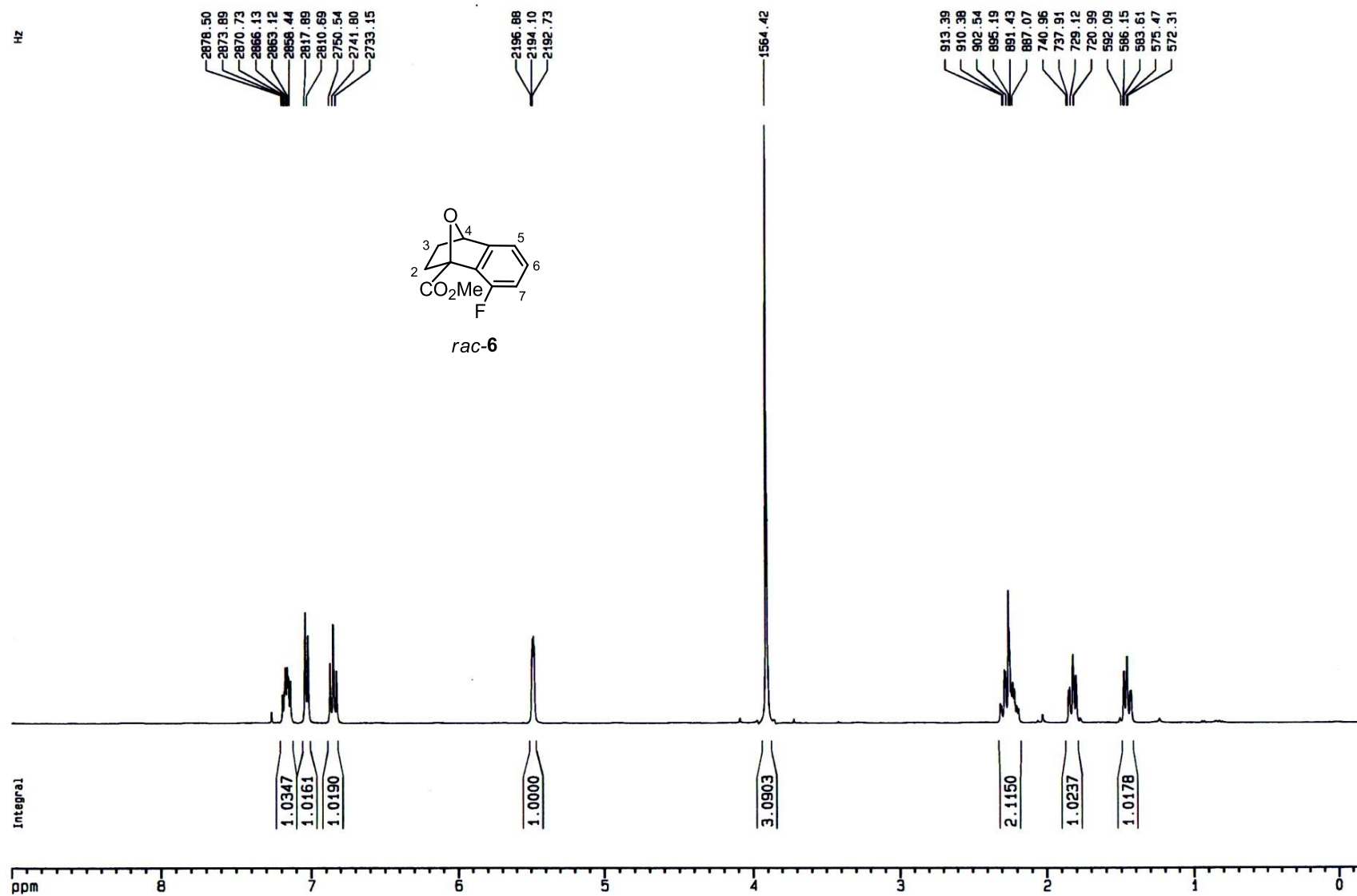


Figure 5. ¹H NMR spectrum of methyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate (*rac*-6).

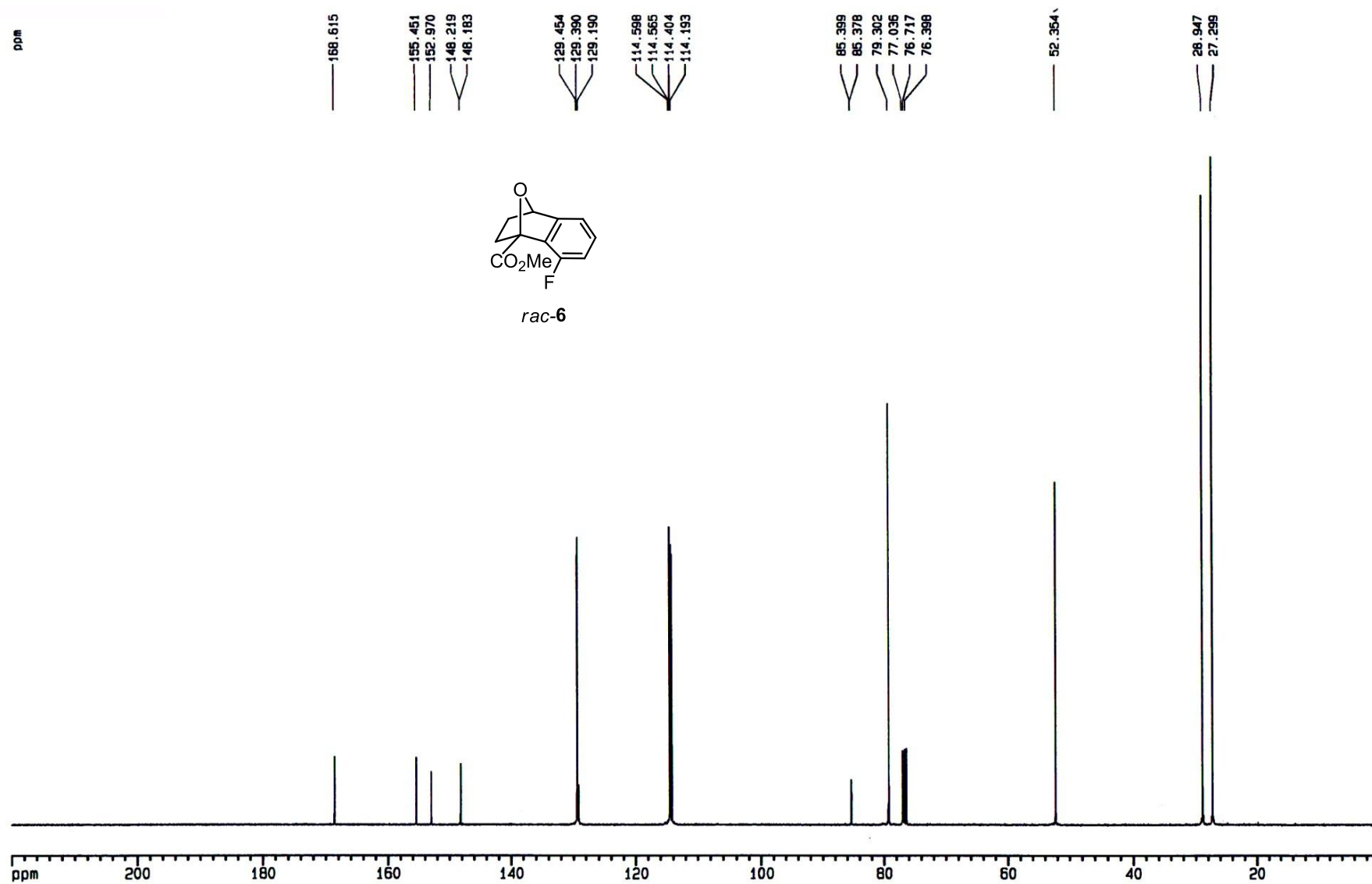


Figure 6. ^{13}C NMR spectrum of methyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate (*rac*-6).

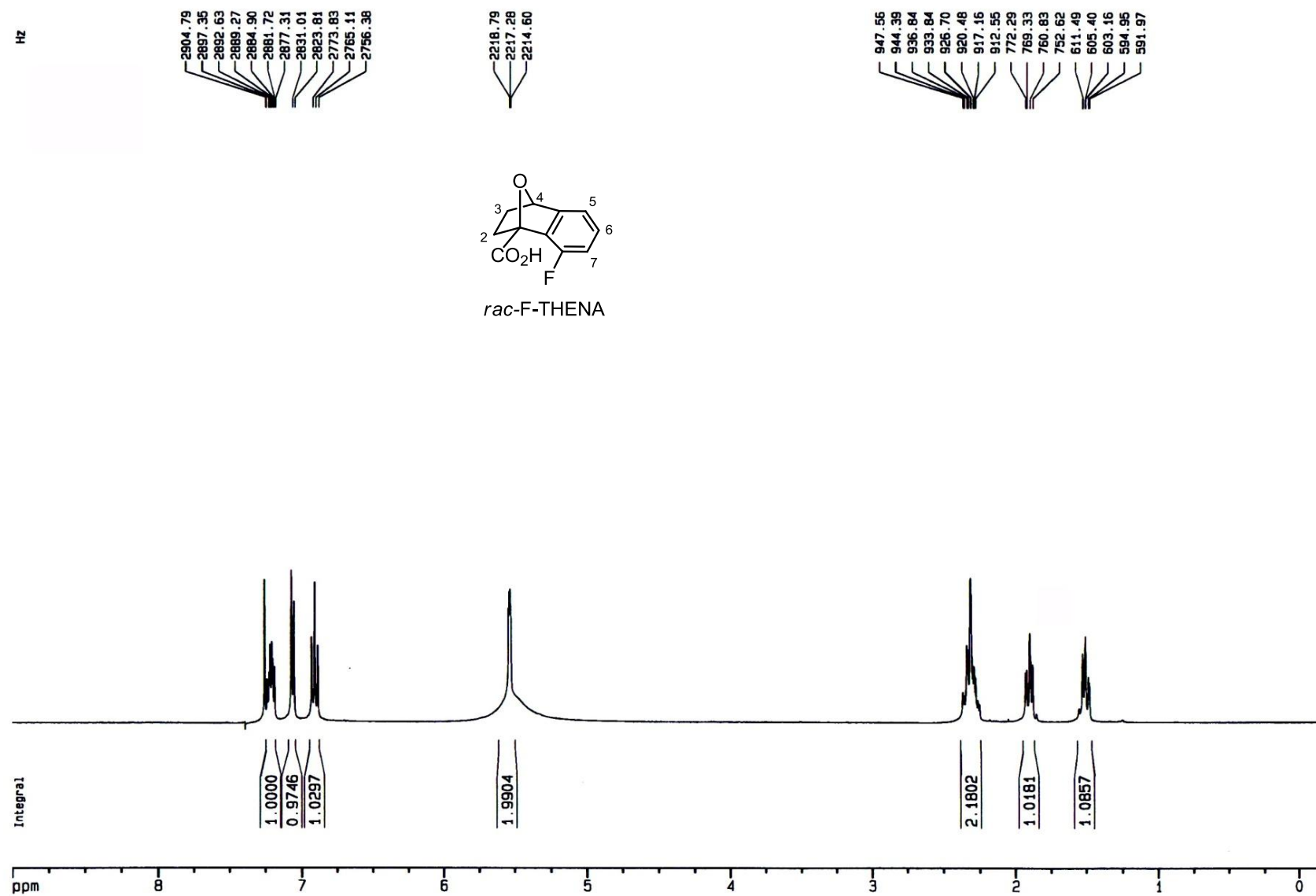


Figure 7. ¹H NMR spectrum of 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylic acid (*rac*-F-THENA).

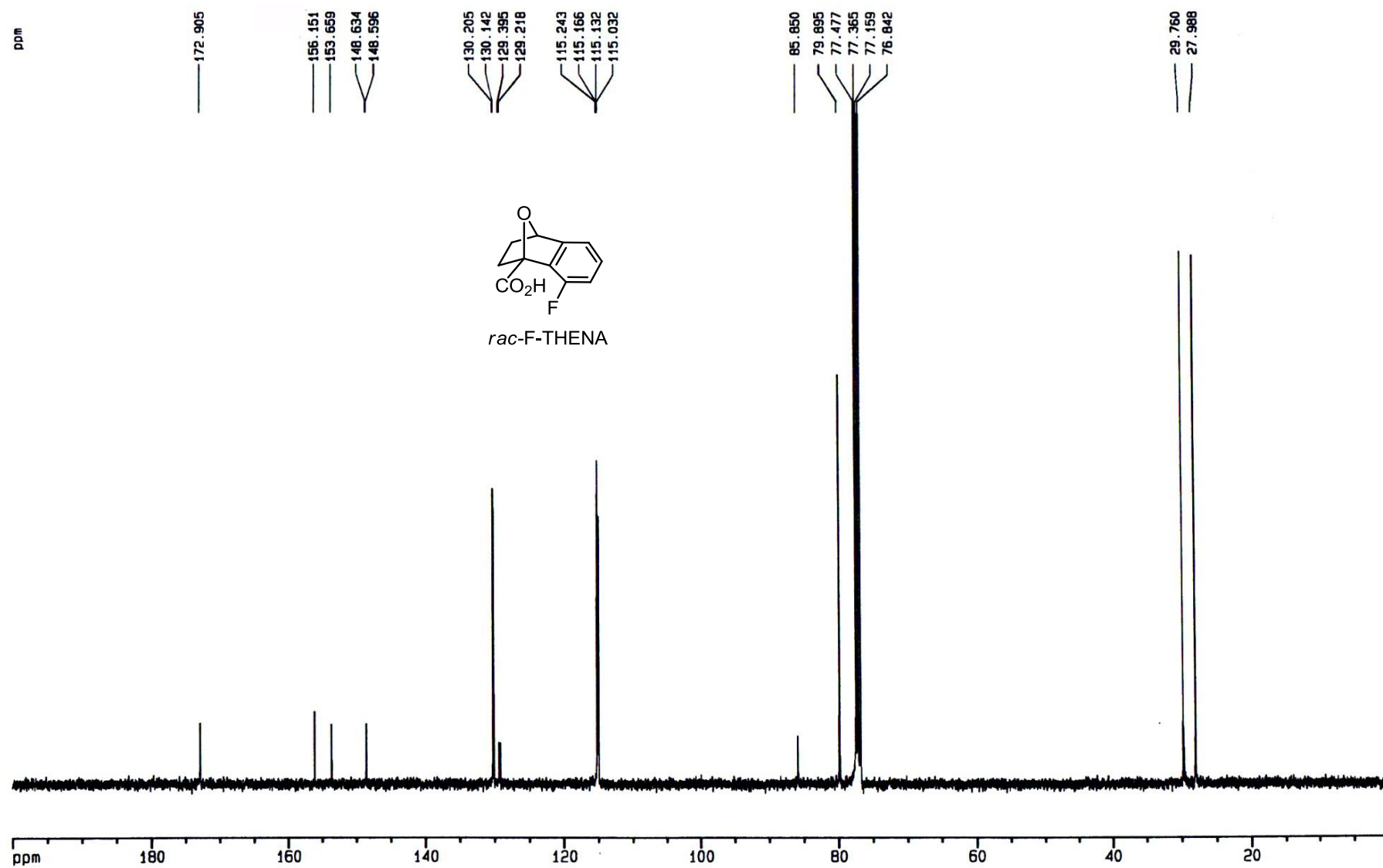


Figure 8. ^{13}C NMR spectrum of 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylic acid (*rac*-F-THENA).

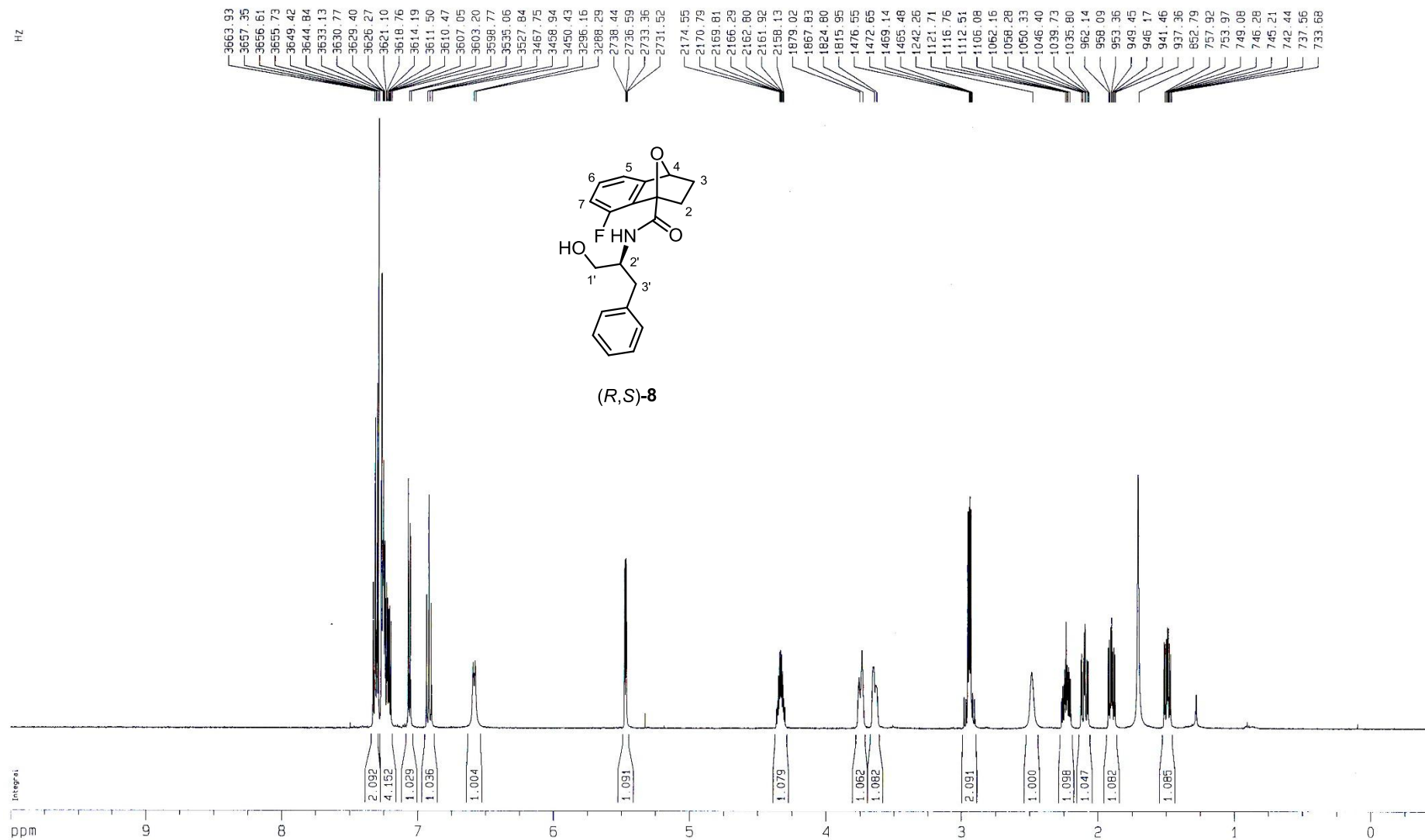


Figure 9. ¹H NMR spectrum of (1*R*,4*S*)-8-fluoro-*N*-((*S*)-1-hydroxy-3-phenylpropan-2-yl)-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxamide ((*R,S*)-**8**).

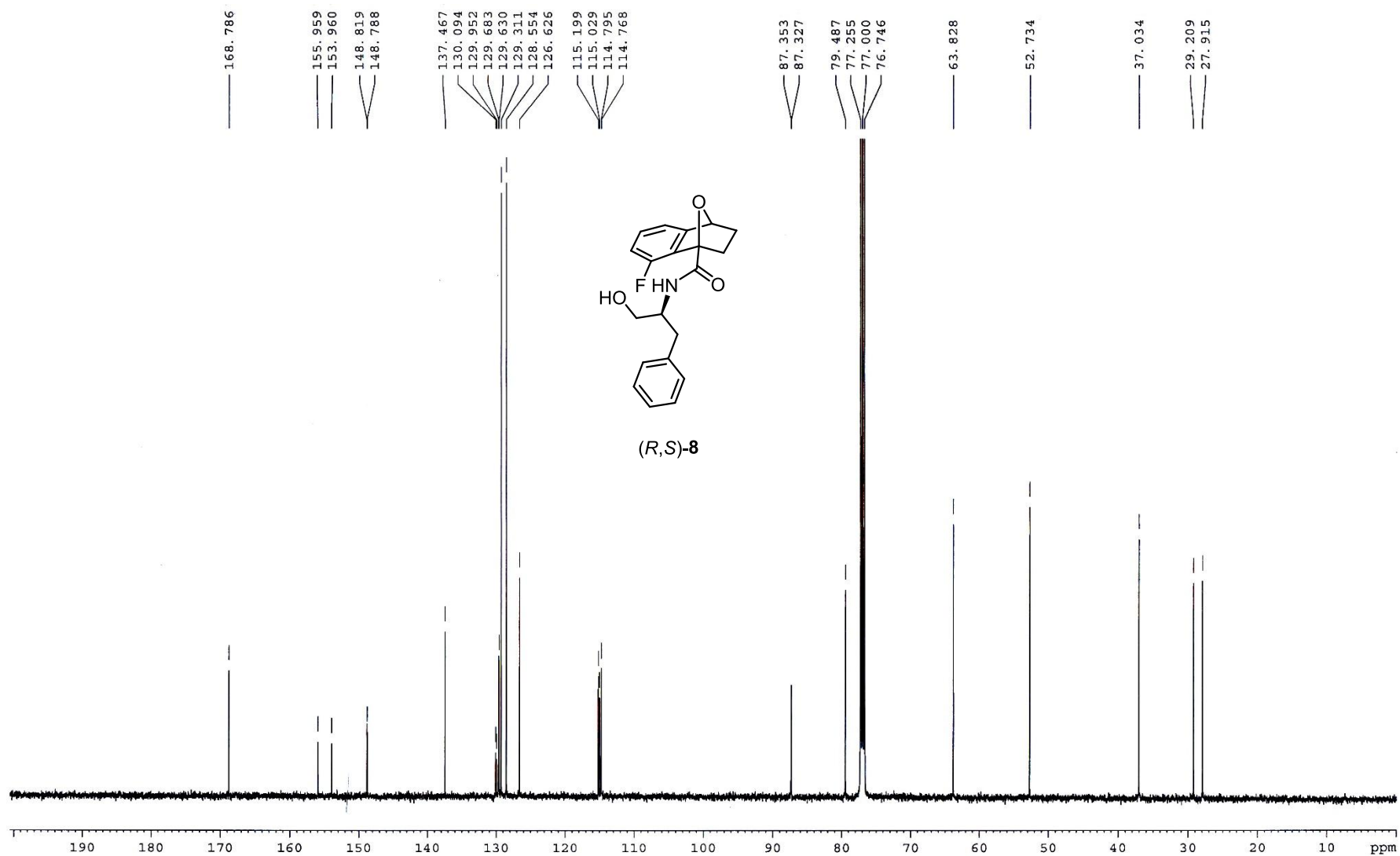


Figure 10. ¹³C NMR spectrum of spectrum of (1*R*,4*S*)-8-fluoro-*N*-((*S*)-1-hydroxy-3-phenylpropan-2-yl)-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxamide ((*R,S*)-**8**).

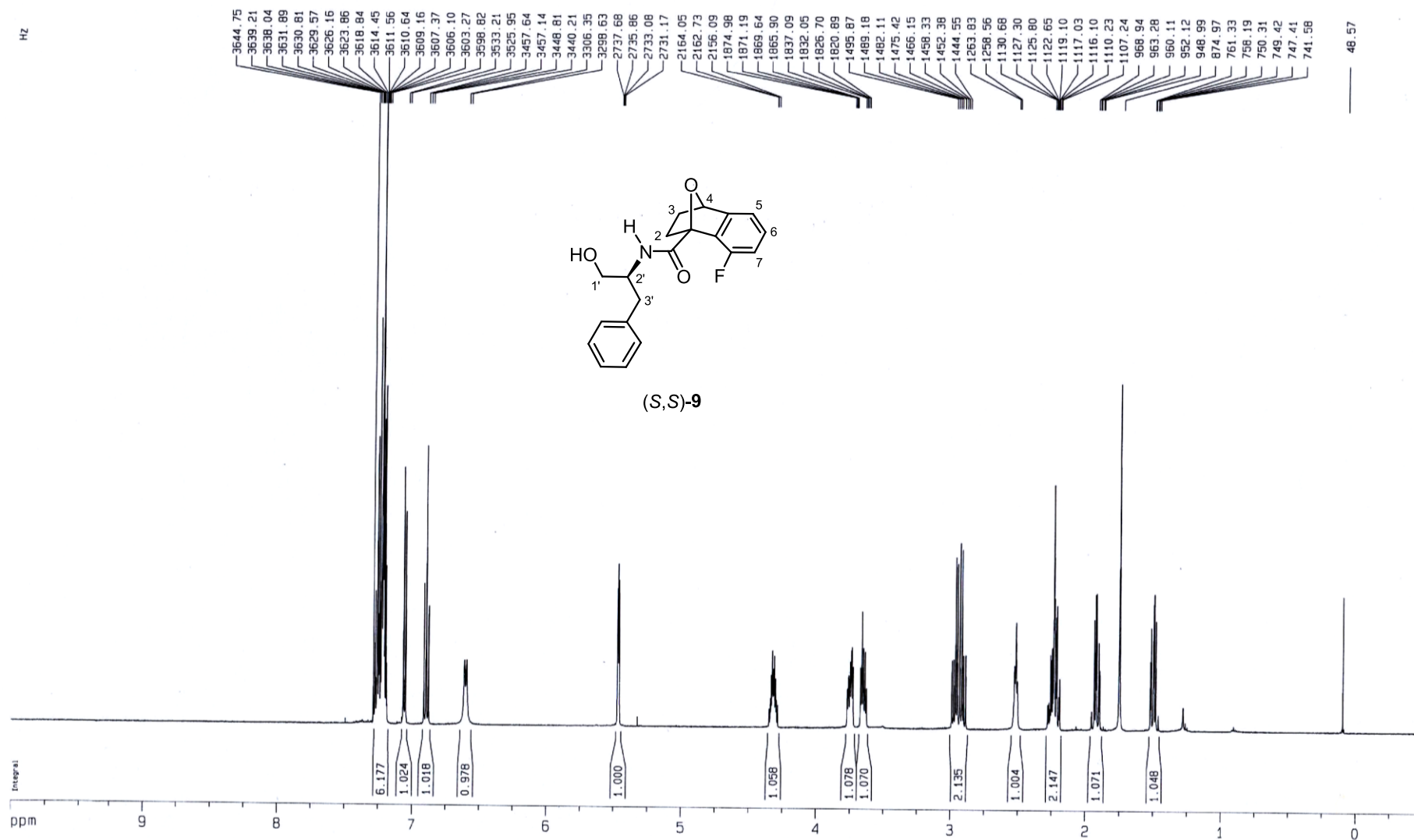


Figure 11. ¹H NMR spectrum of (1*S*,4*R*)-8-fluoro-*N*-((*S*)-1-hydroxy-3-phenylpropan-2-yl) - 1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxamide ((*S,S*)-**9**).

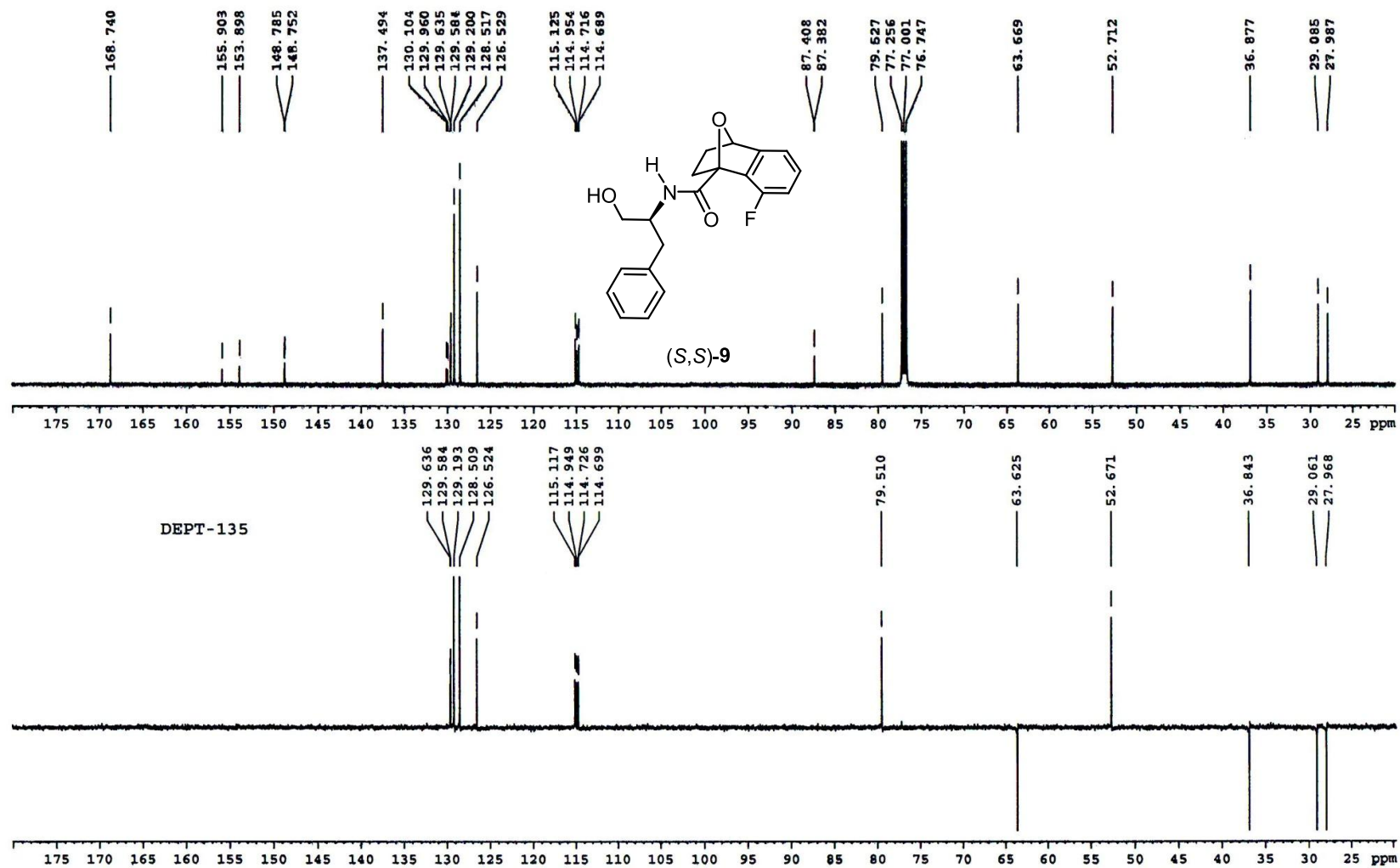


Figure 12. ^{13}C NMR spectra of (1*S*,4*R*)-8-fluoro-*N*-((*S,S*)-1-hydroxy-3-phenylpropan-2-yl)-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxamide ((*S,S*)-**9**).

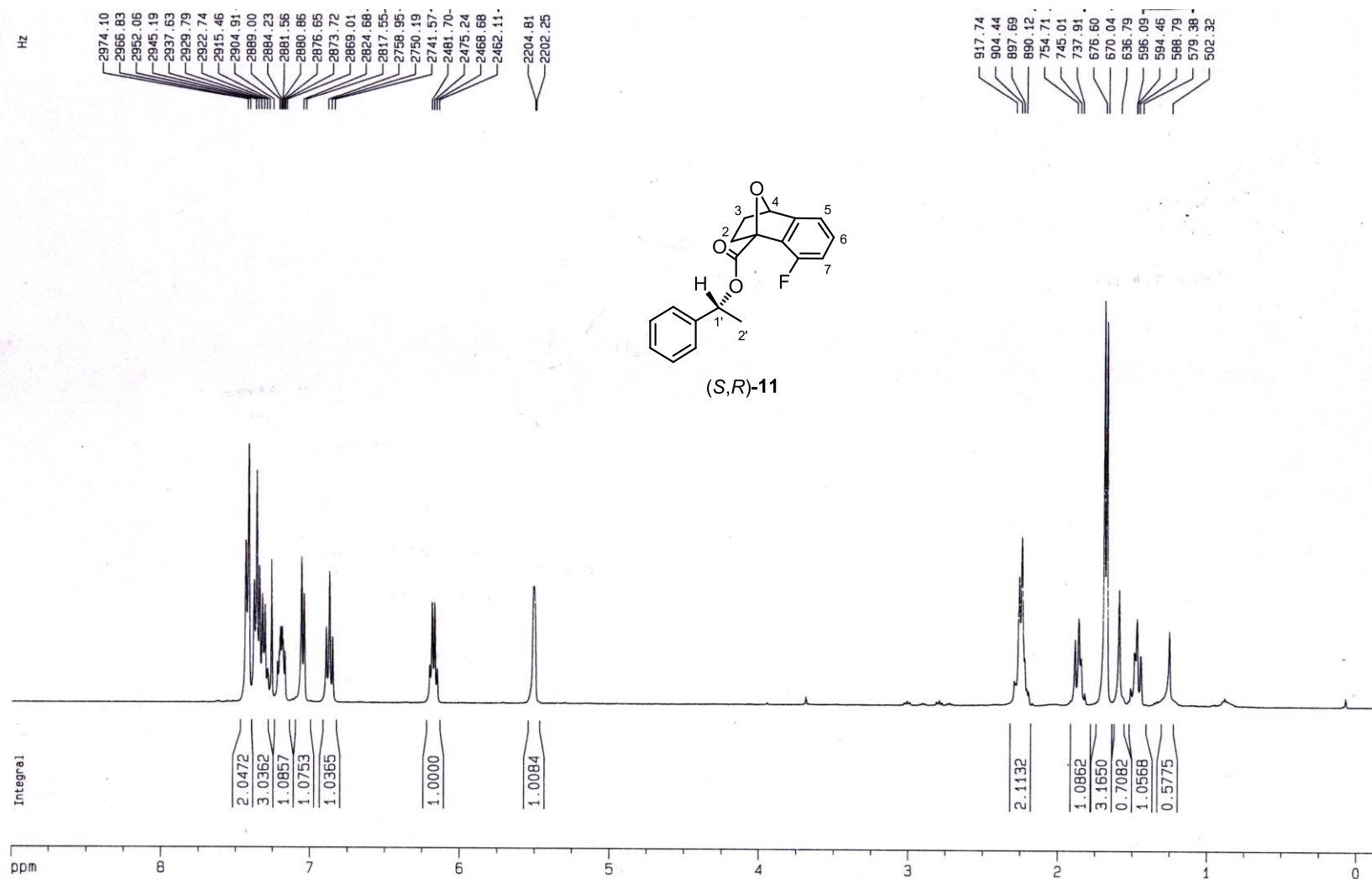


Figure 13. ¹H NMR spectrum of (1*S*,4*R*)-(*R*)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S*,*R*)-11).

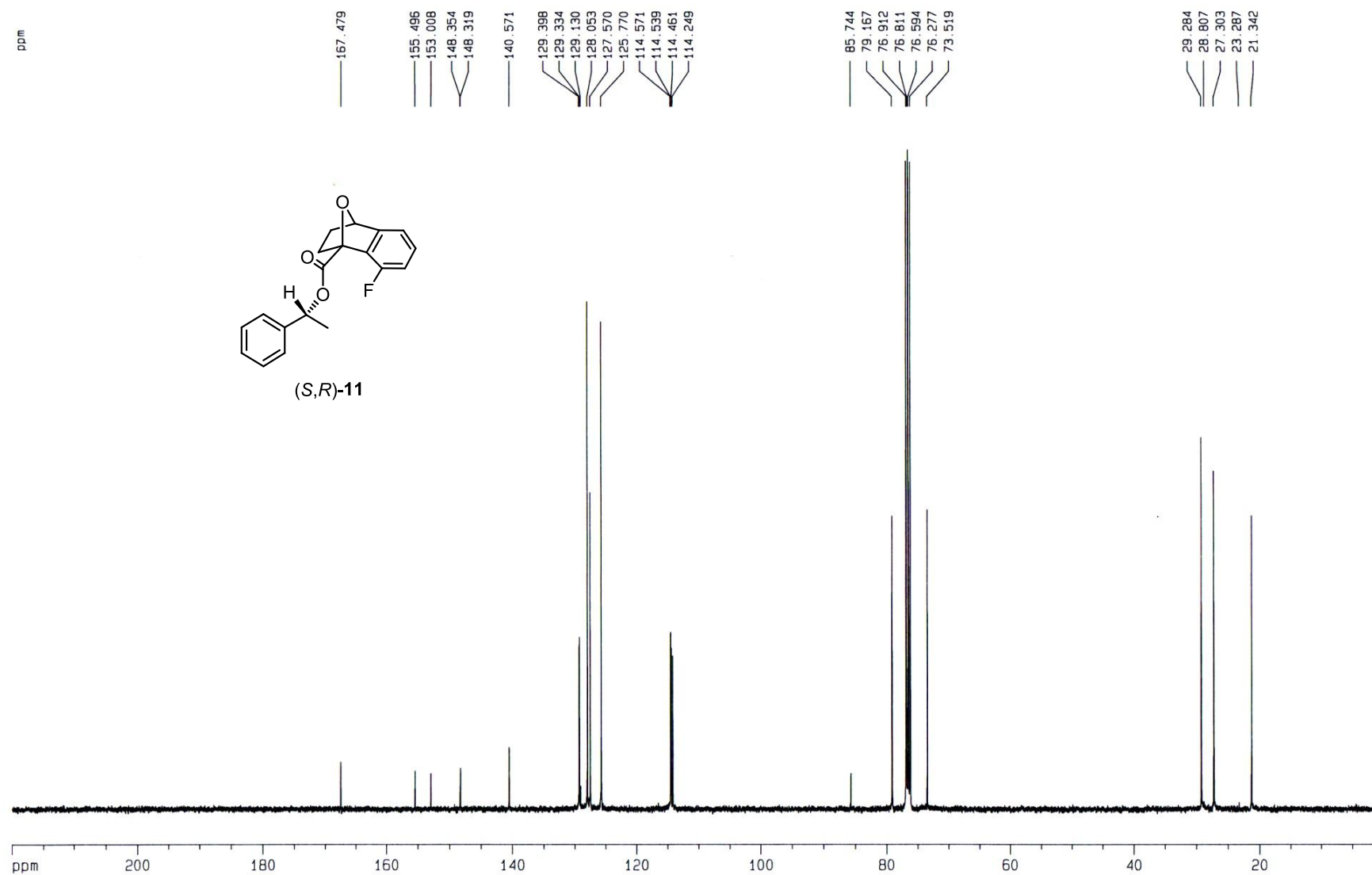


Figure 14. ^{13}C NMR spectrum of (1*S*,4*R*)-(1*R*)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,R*)-11).

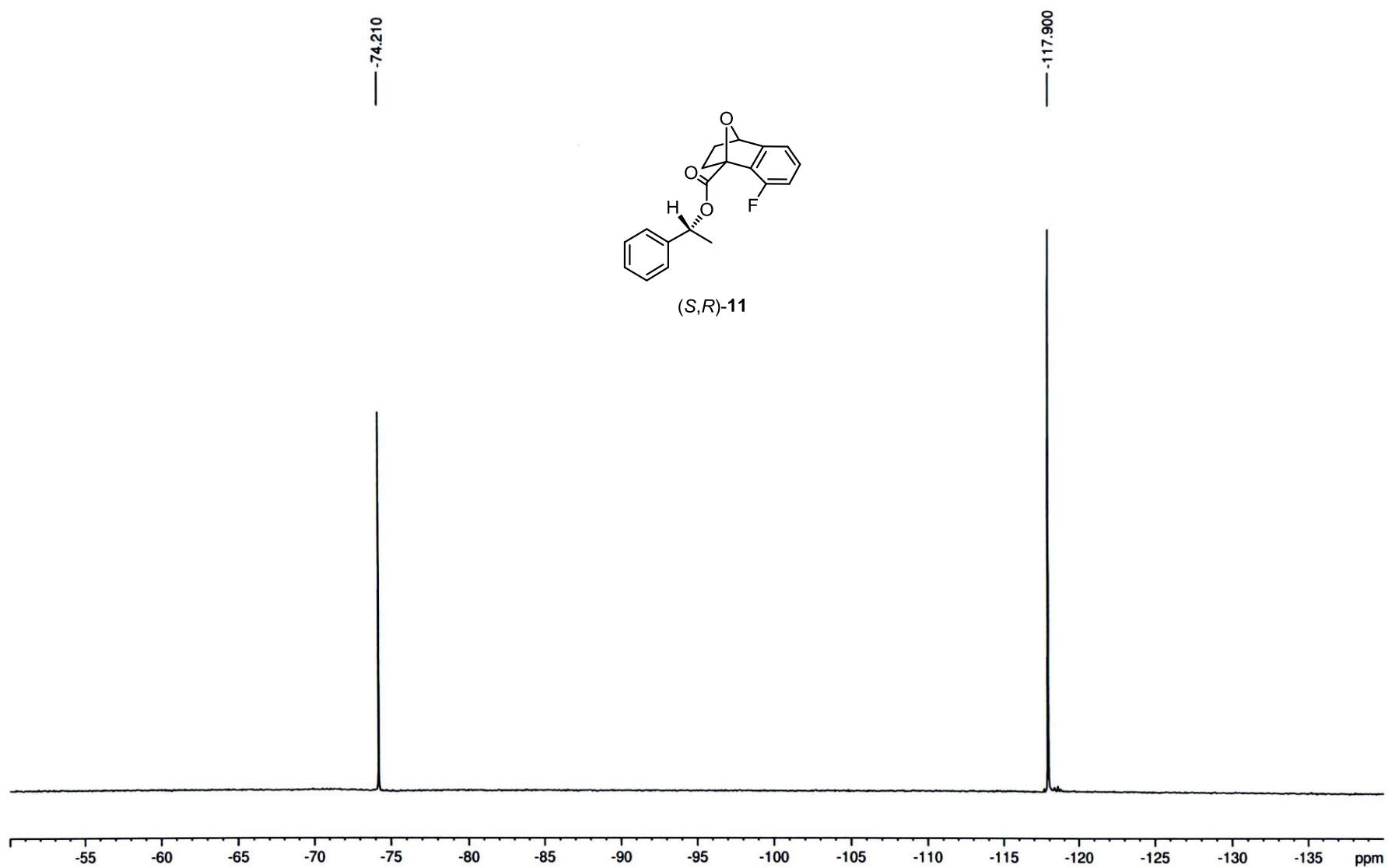


Figure 15. ^{19}F NMR spectrum of (1S,4R)-(R)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,R)-11).

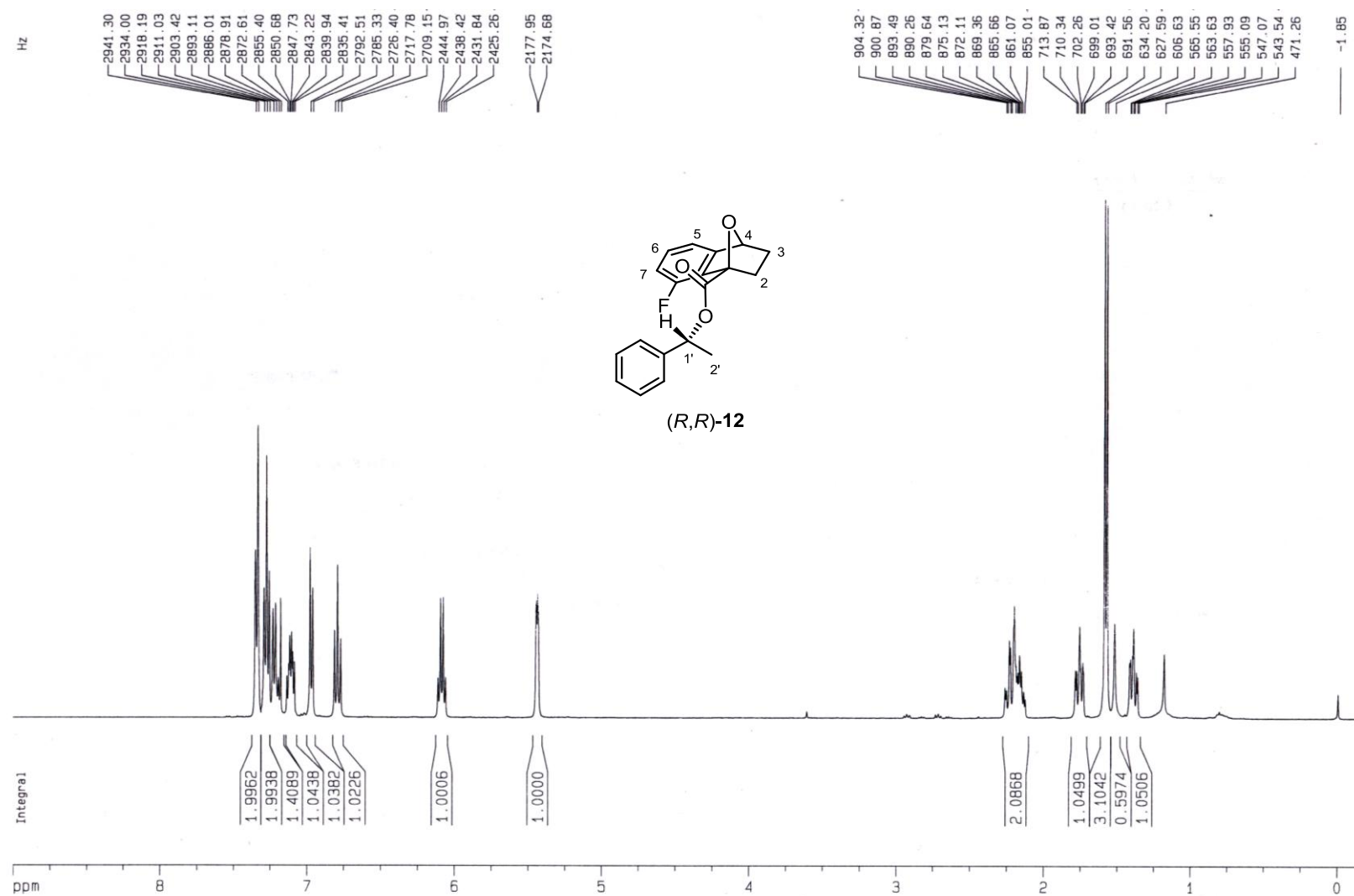


Figure 16. ¹H NMR spectrum of (1*R*,4*S*)-(1*R*)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,R*)-12).

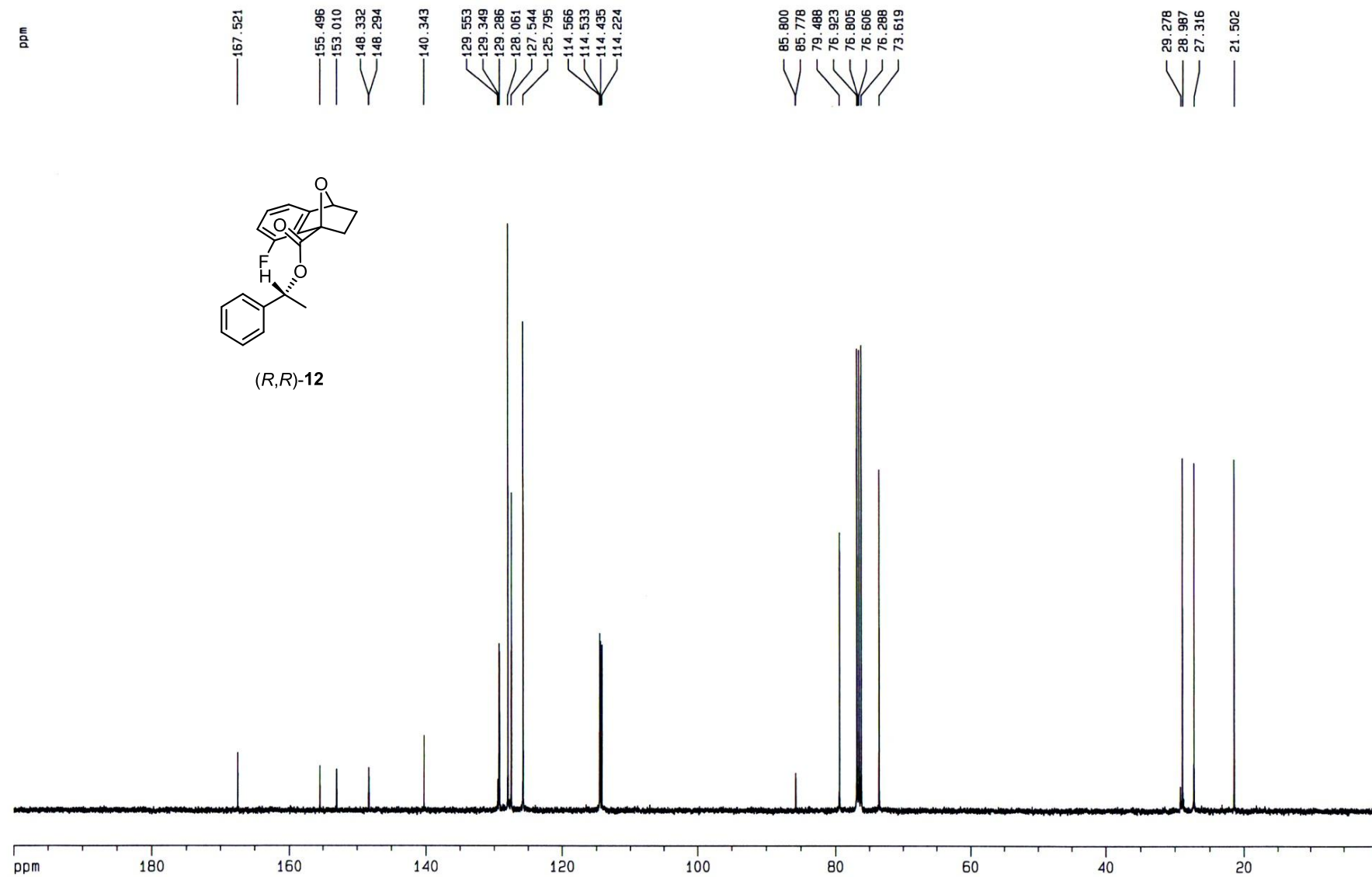
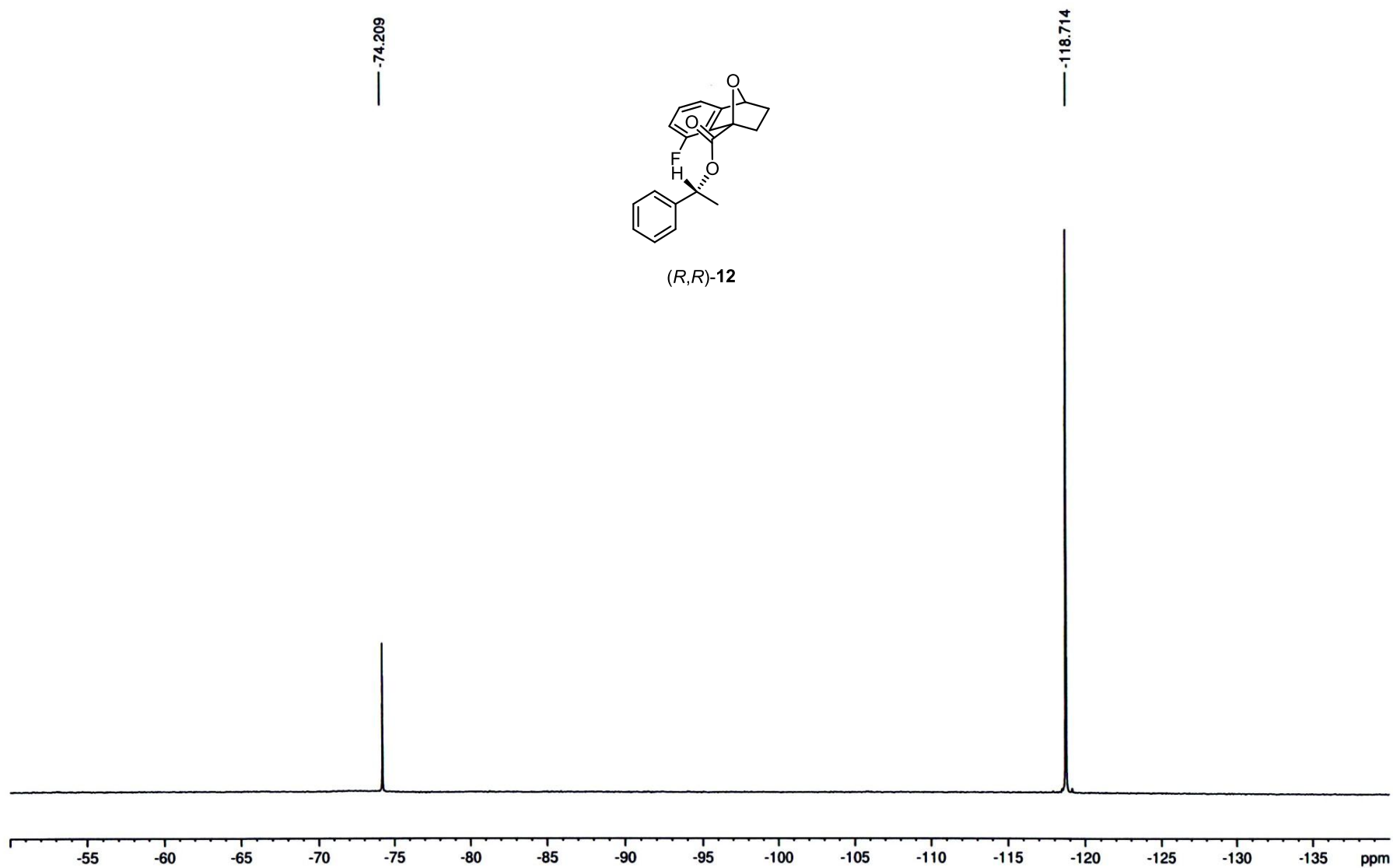


Figure 17. ¹³C NMR spectrum of (1*R*,4*S*)-(1*R*)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,R*)-12).



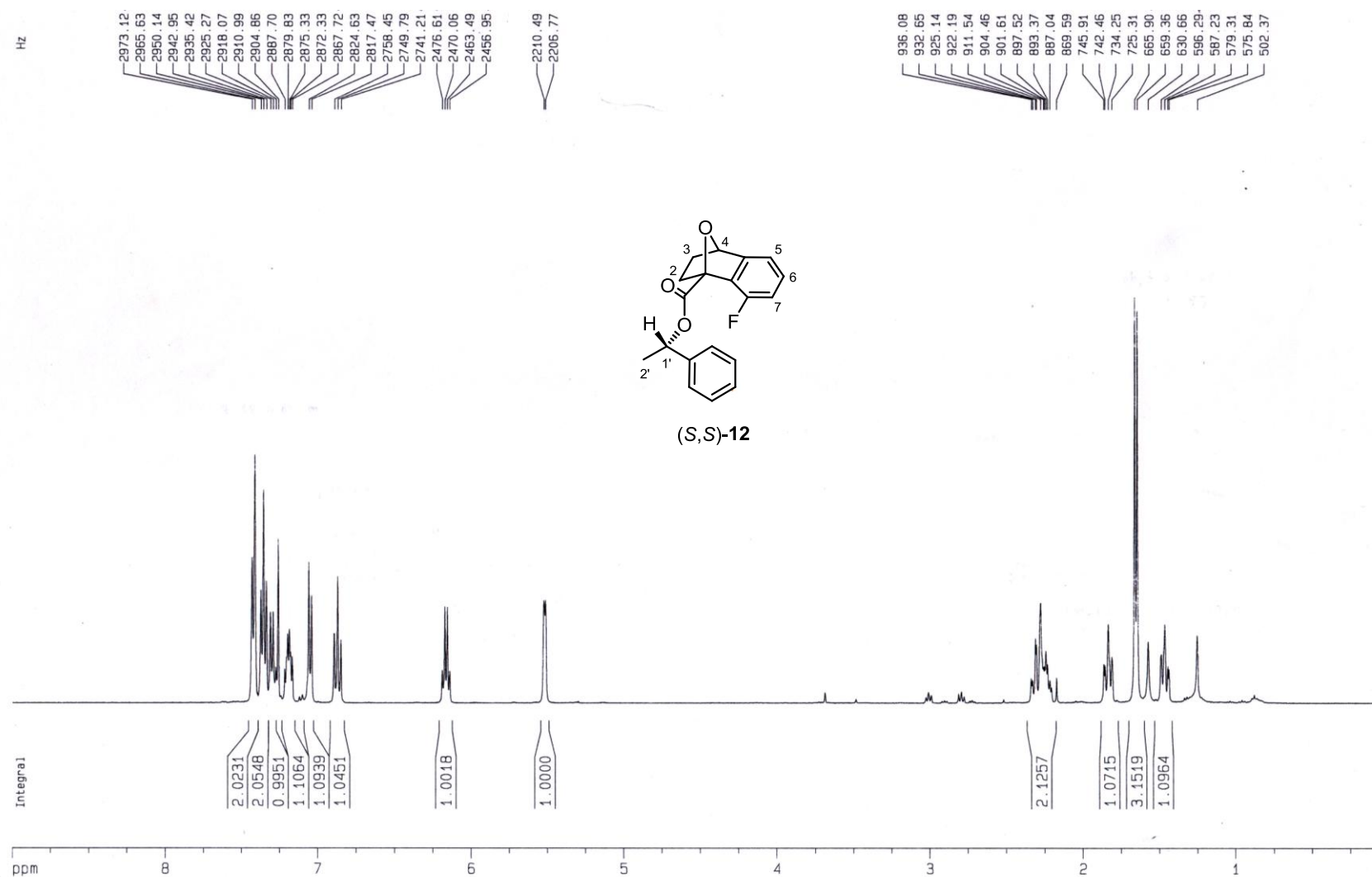


Figure 19. ¹H NMR spectrum of (1*S*,4*R*)-(S)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,S)-12).

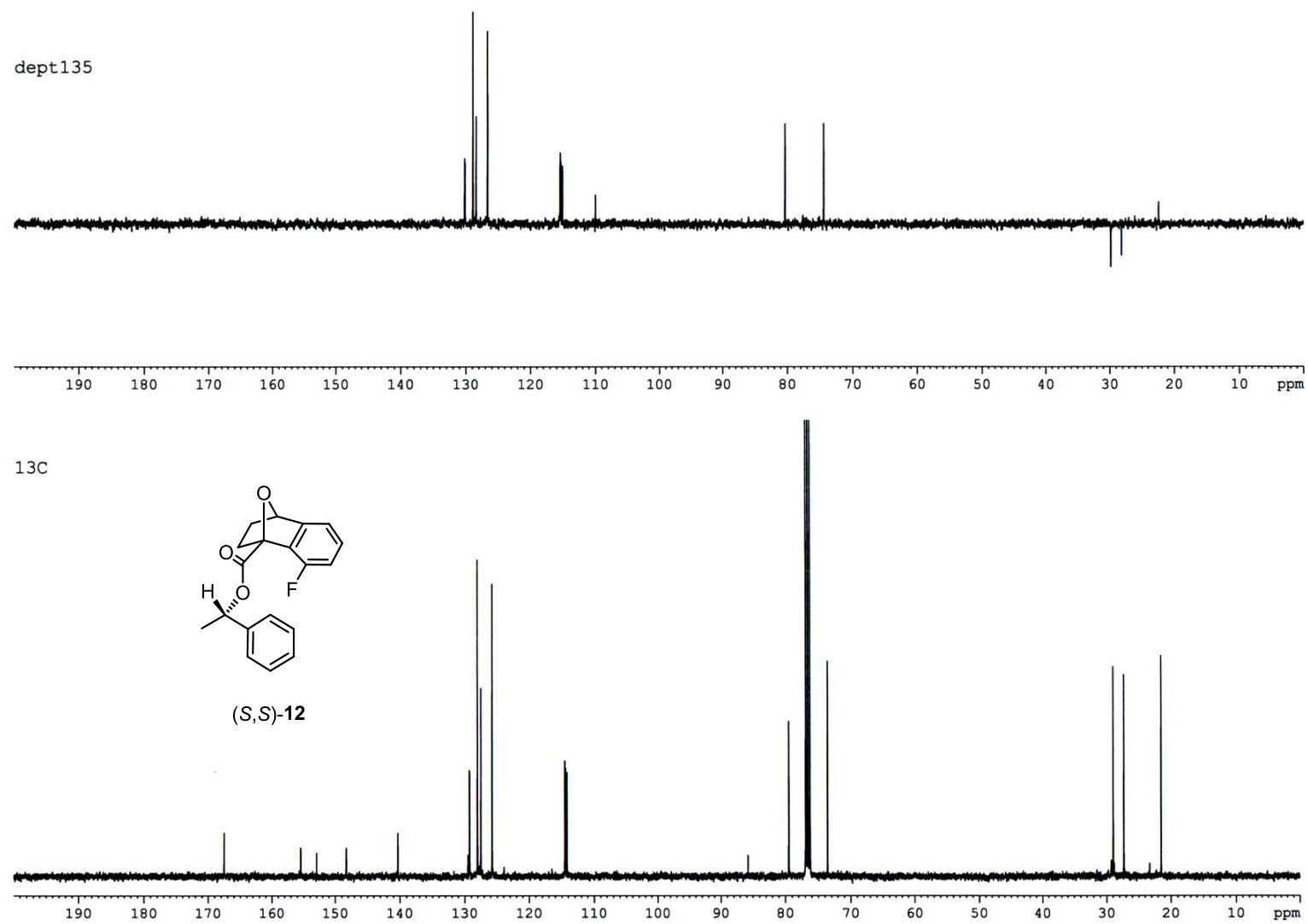


Figure 20. ^{13}C NMR spectra of (1*S*,4*R*)-(S)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,S)-12).

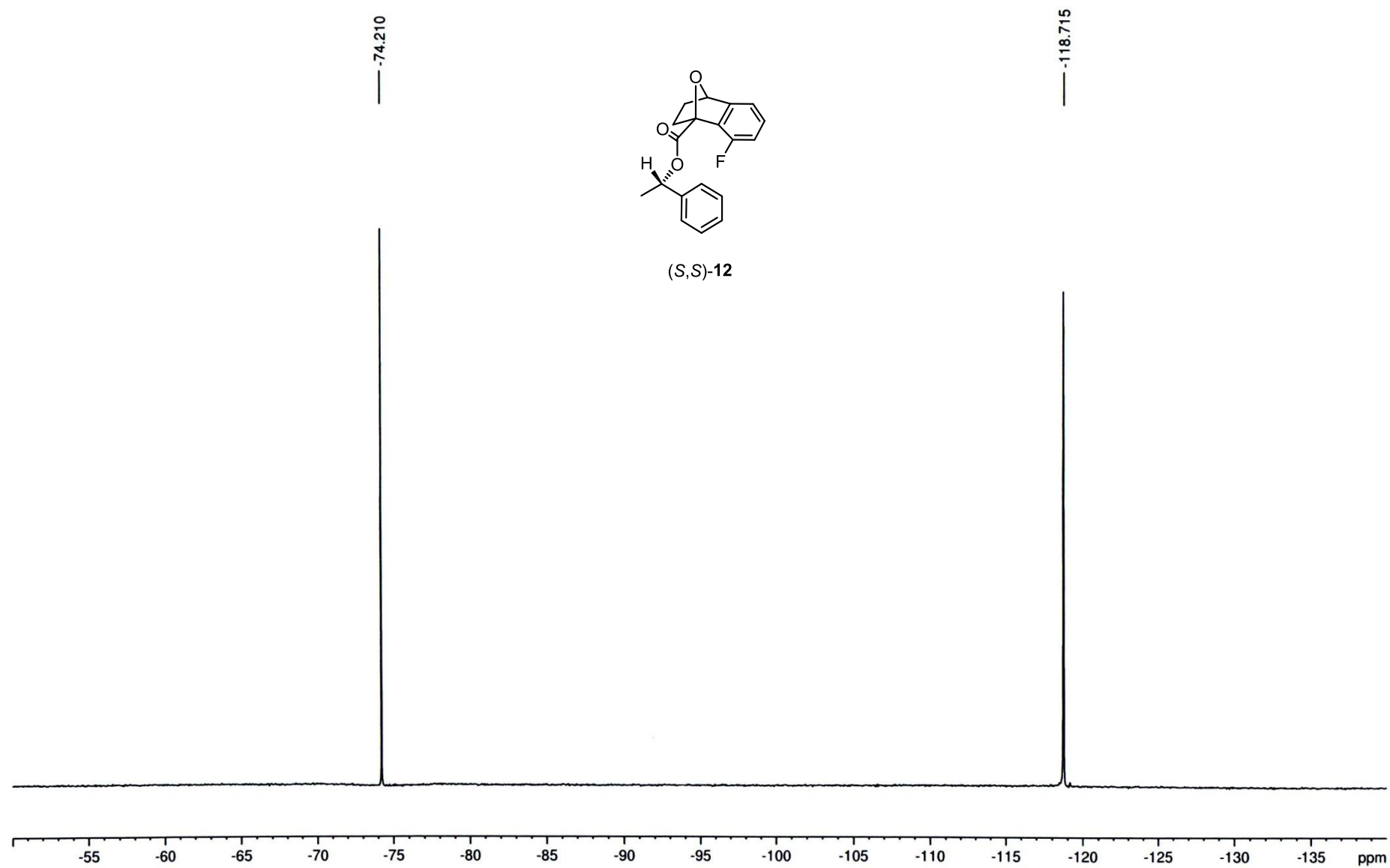


Figure 21. ^{19}F NMR spectrum of (1*S*,4*R*)-(S)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,S)-12).

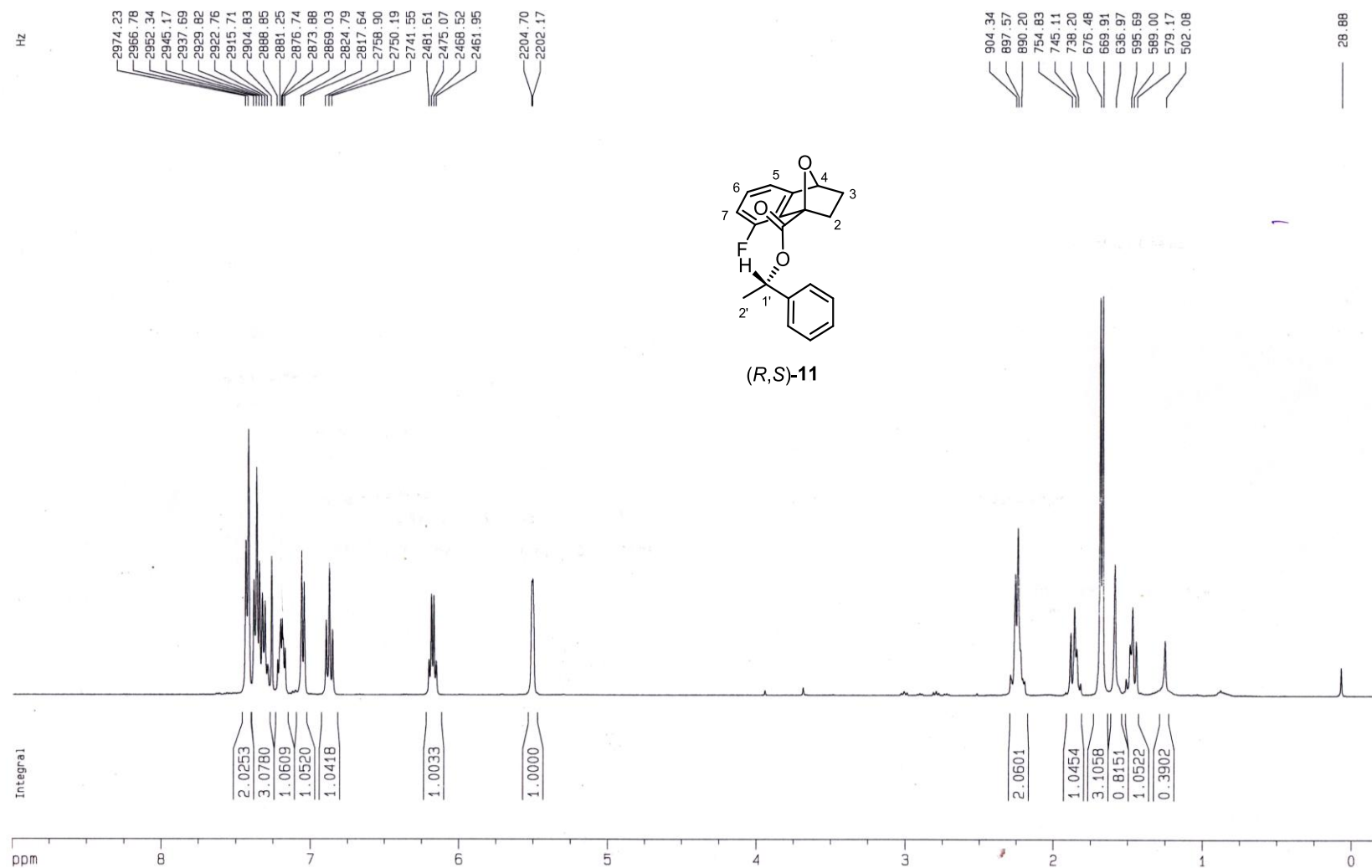


Figure 22. ¹H NMR spectrum of (1*R*,4*S*)-(S)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-11).

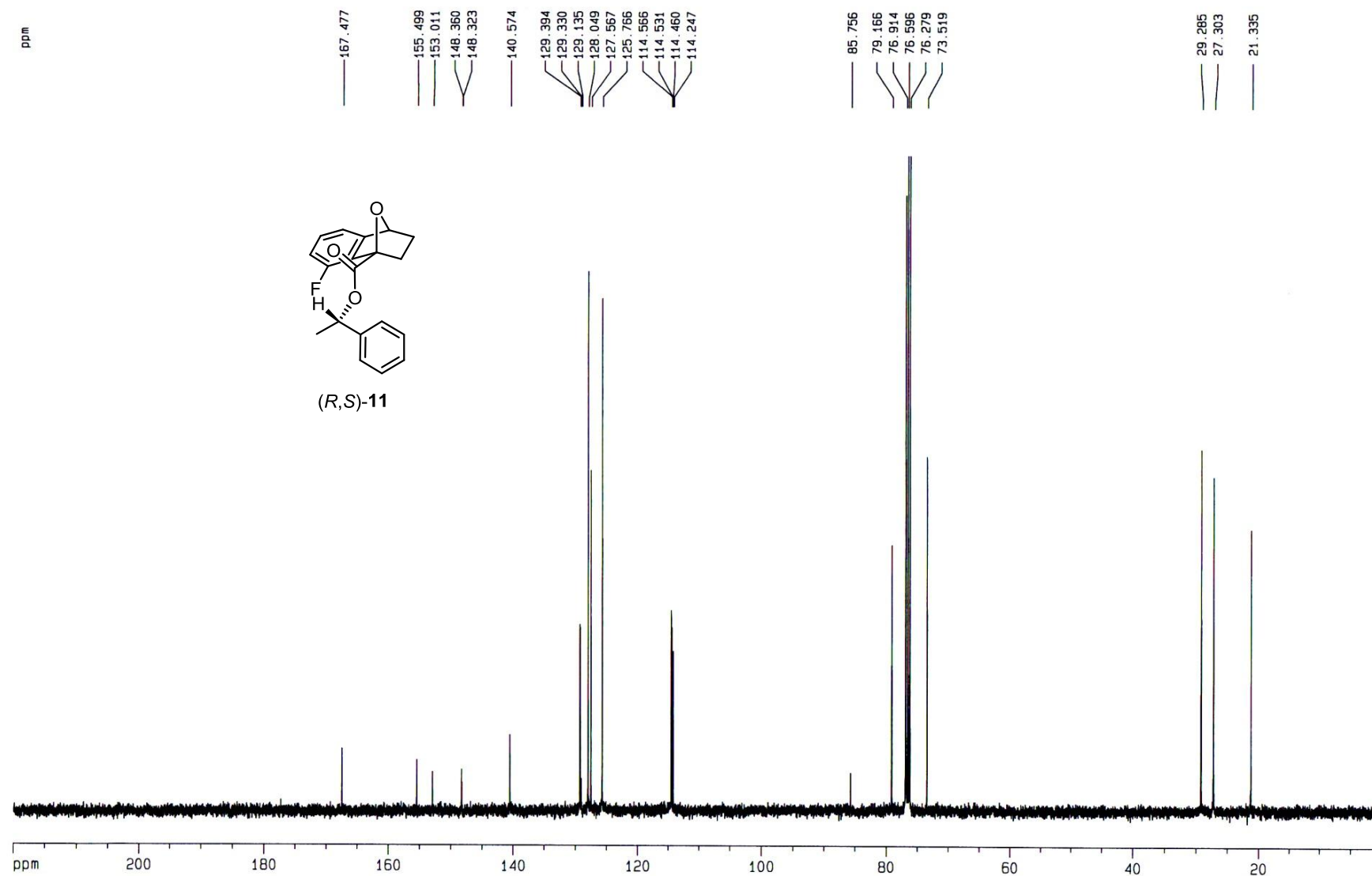


Figure 23. ^1H NMR spectrum of (1*R*,4*S*)-(S)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-11).

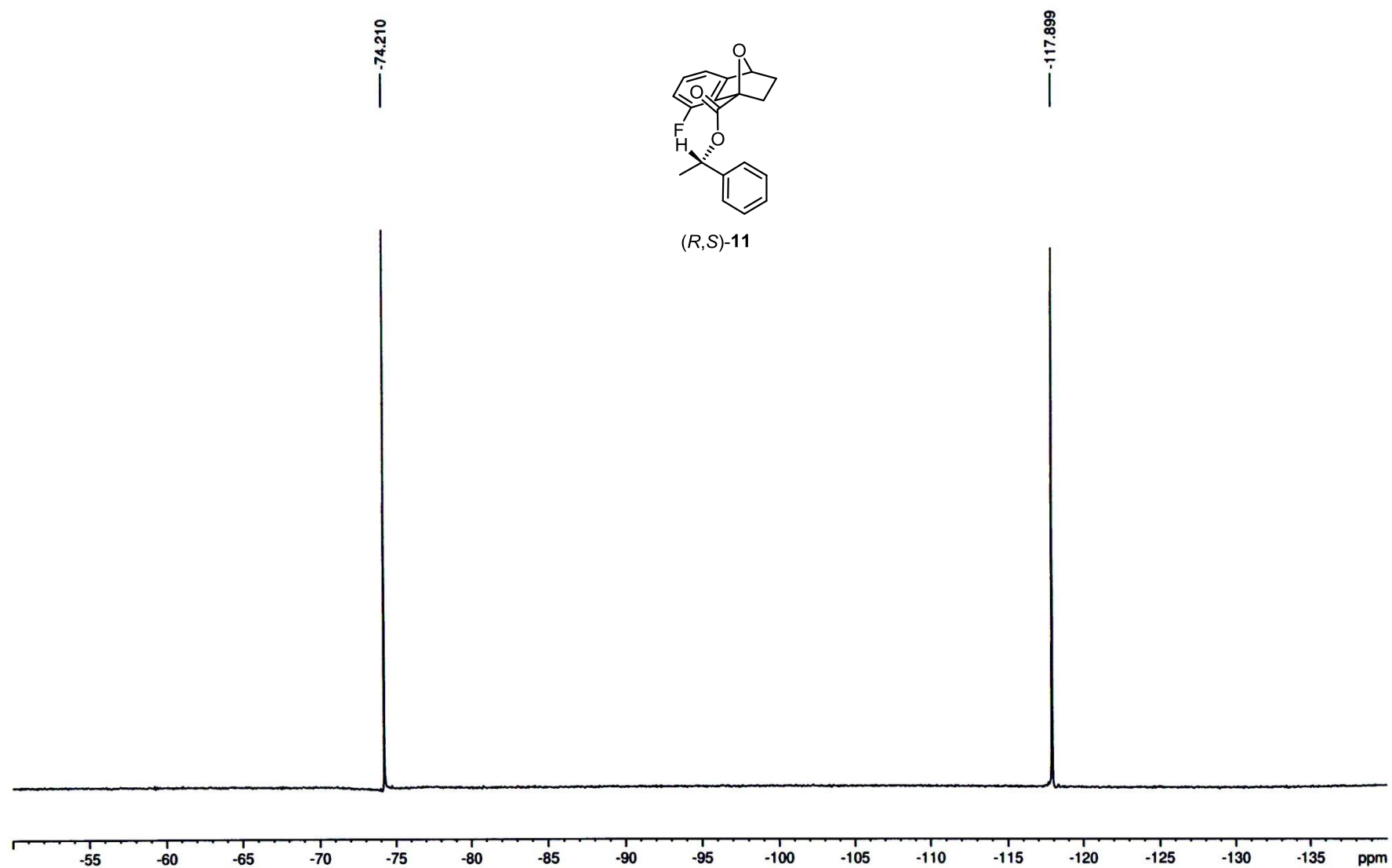


Figure 24. ^{19}F NMR spectrum of (1R,4S)-(S)-1-phenylethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((R,S)-11).

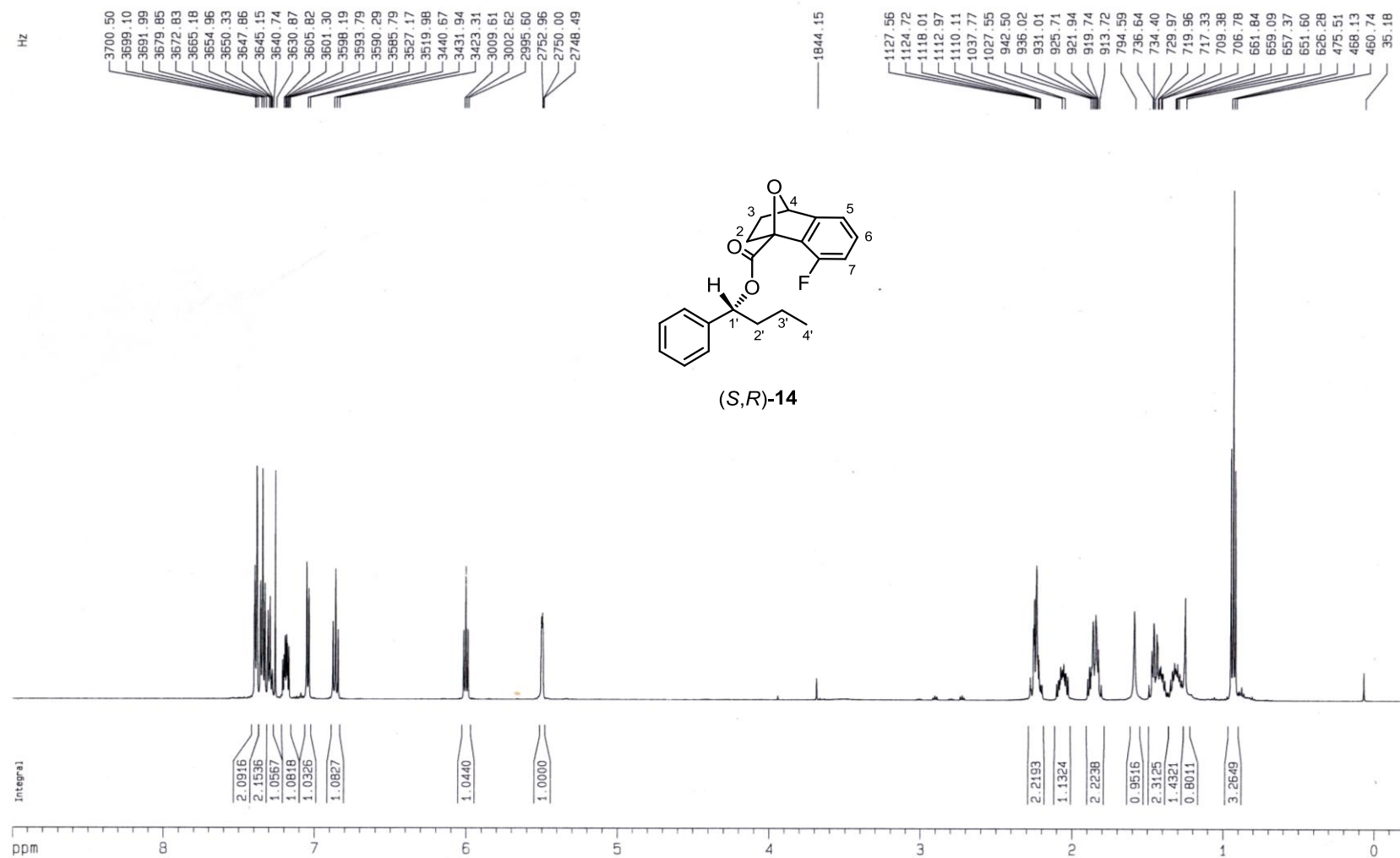


Figure 25. ¹H NMR spectrum of (1*S*,4*R*)-(R)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S*,*R*)-14).

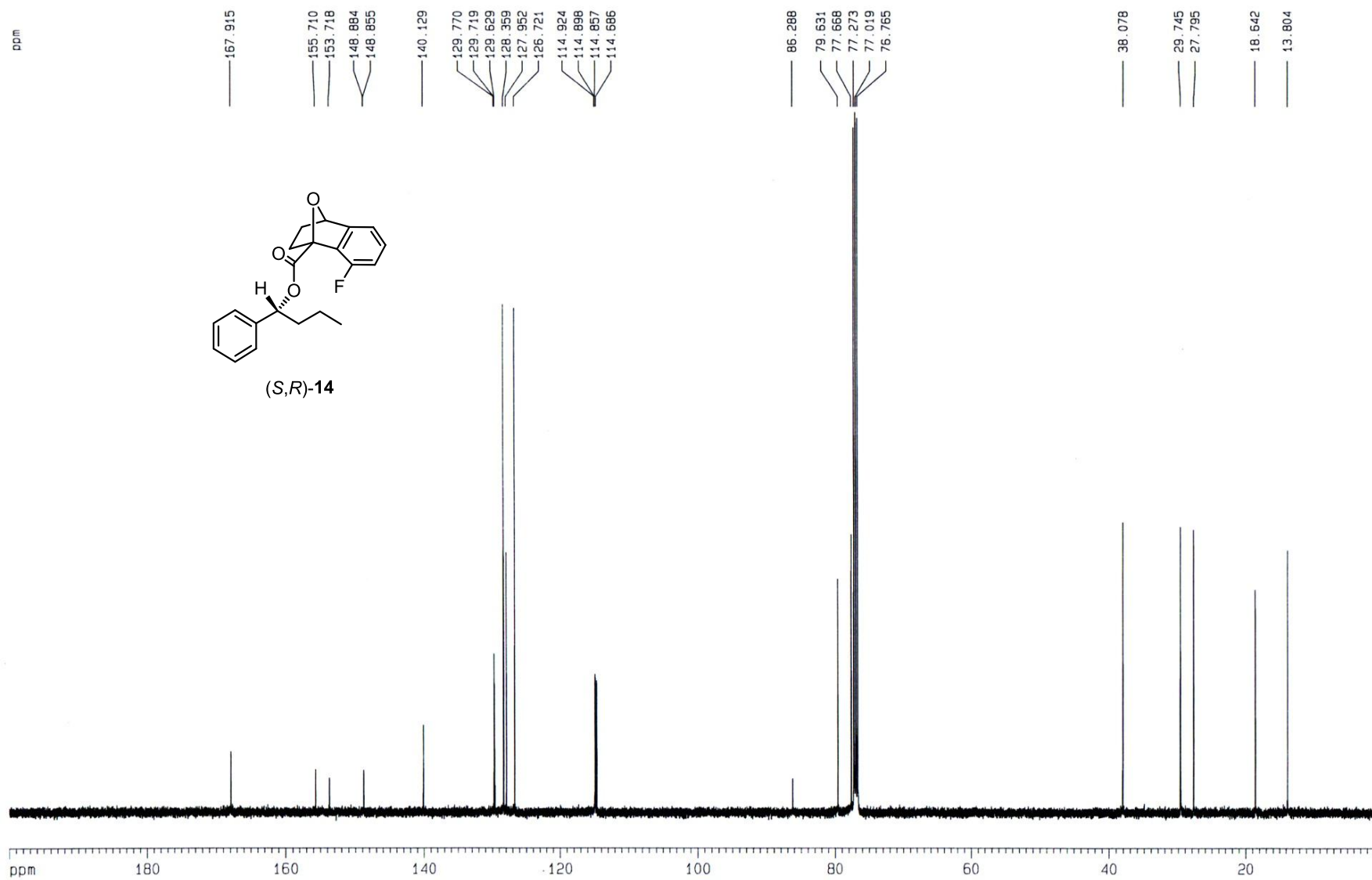


Figure 26. ^{13}C NMR spectrum of (1*S*,4*R*)-(R)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,R)-14).

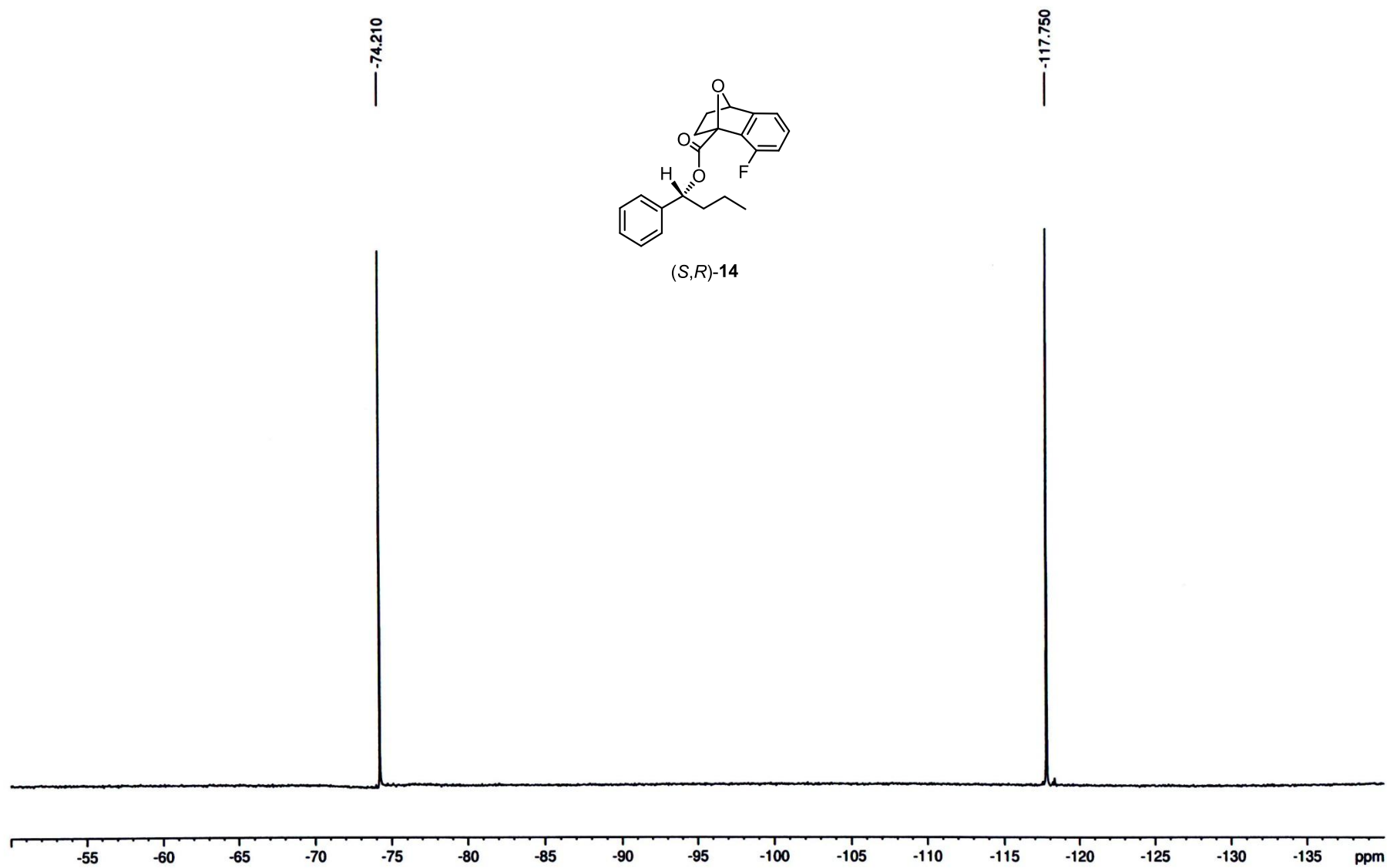


Figure 27. ^{19}F NMR spectrum of (1S,4R)-(R)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,R)-14).

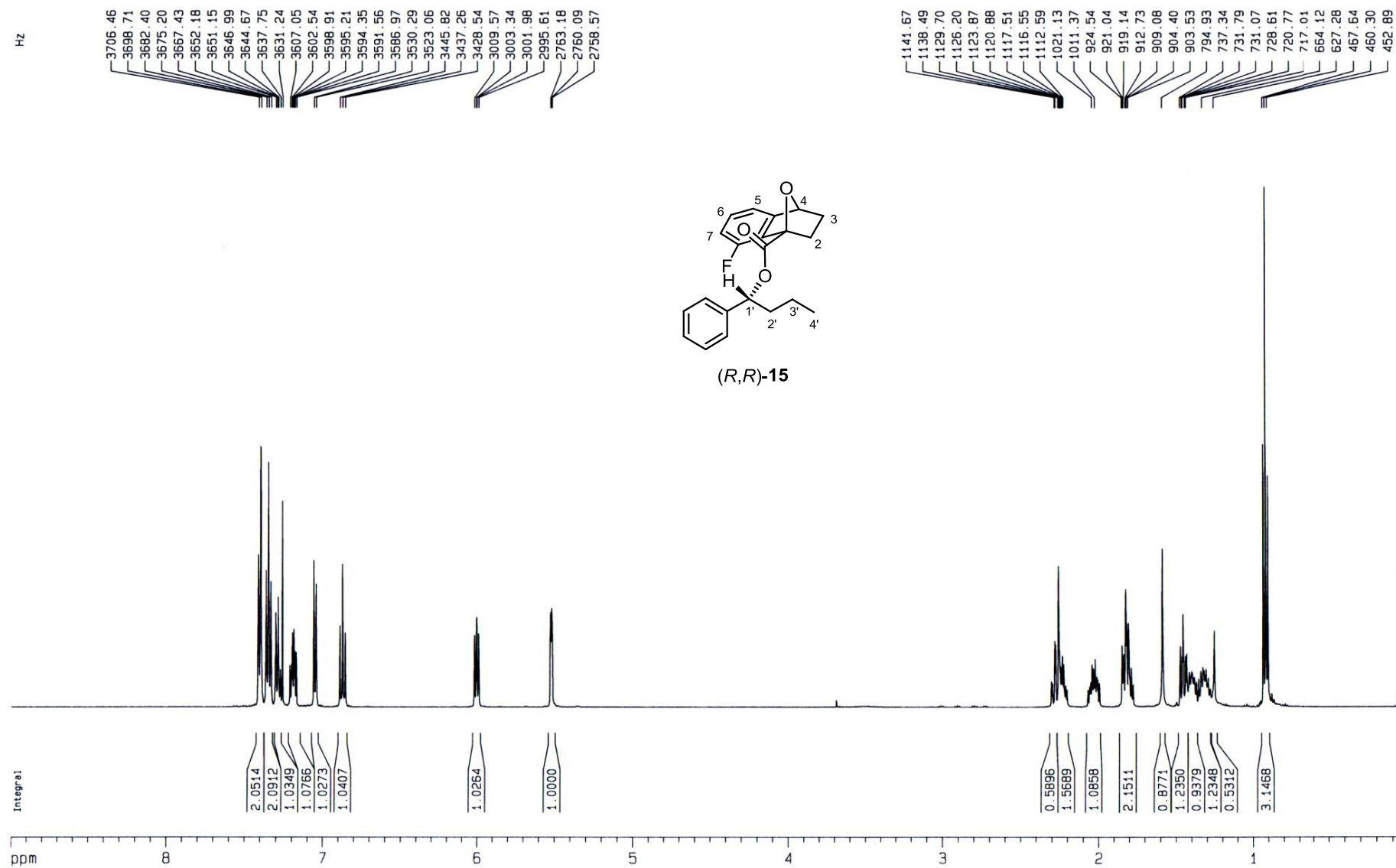


Figure 28. ^1H NMR spectrum of (1*R*,4*S*)-(*R*)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,R*)-15).

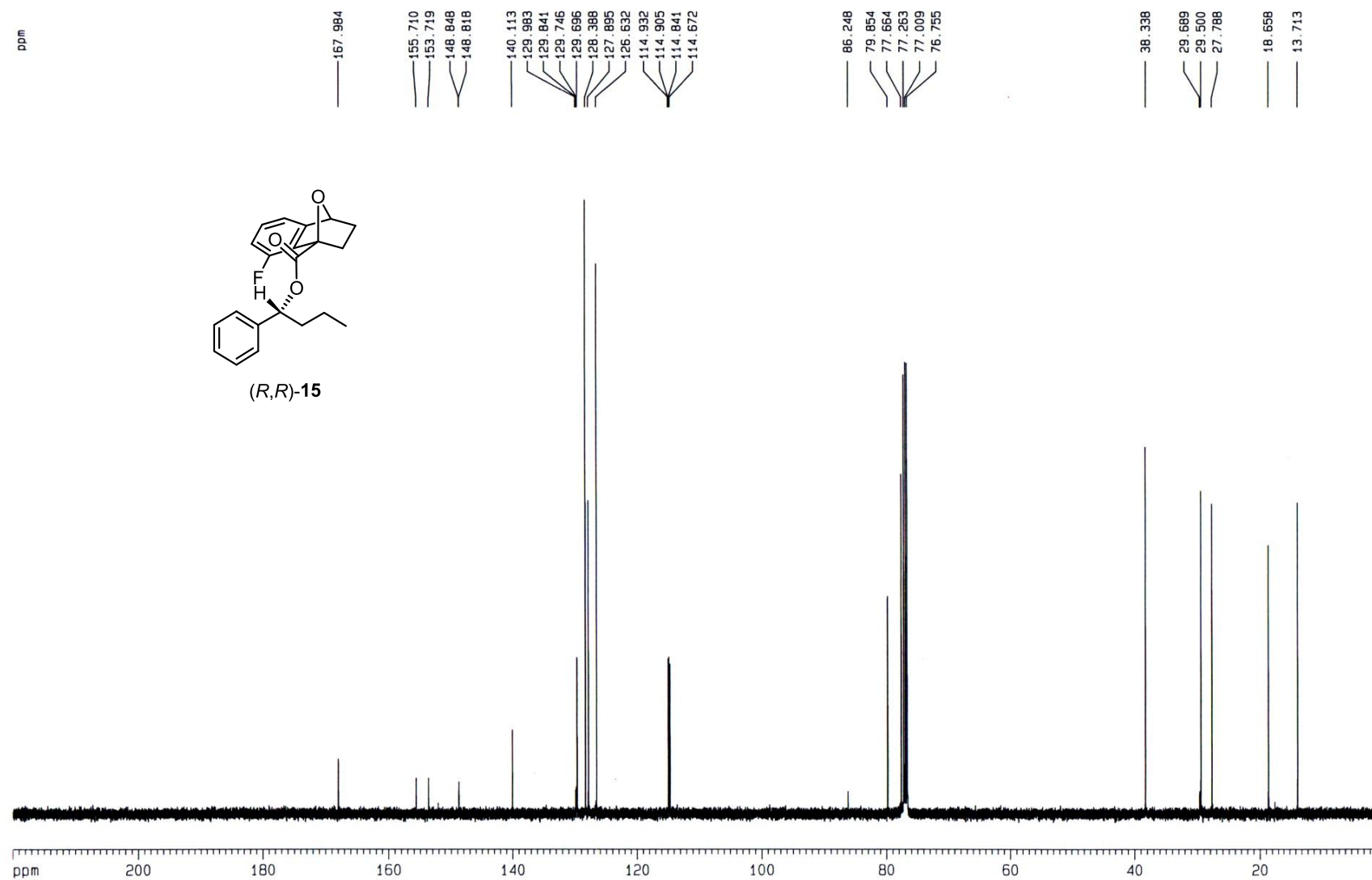


Figure 29. ¹³C NMR spectrum of (1*R*,4*S*)-(R)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,R*)-15).

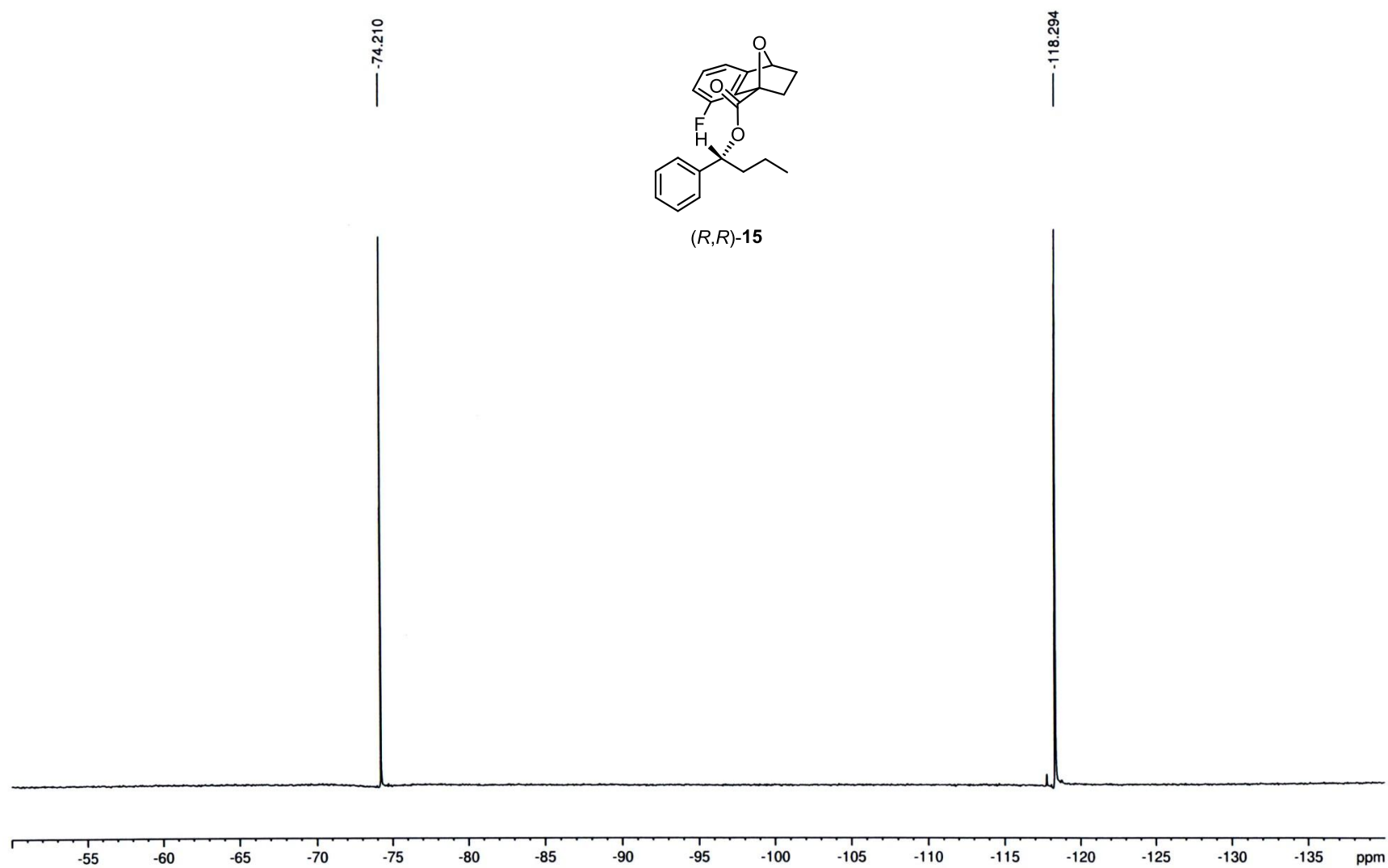


Figure 30. ^{19}F NMR spectrum of (1*R*,4*S*)-(R)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((R,R)-15).

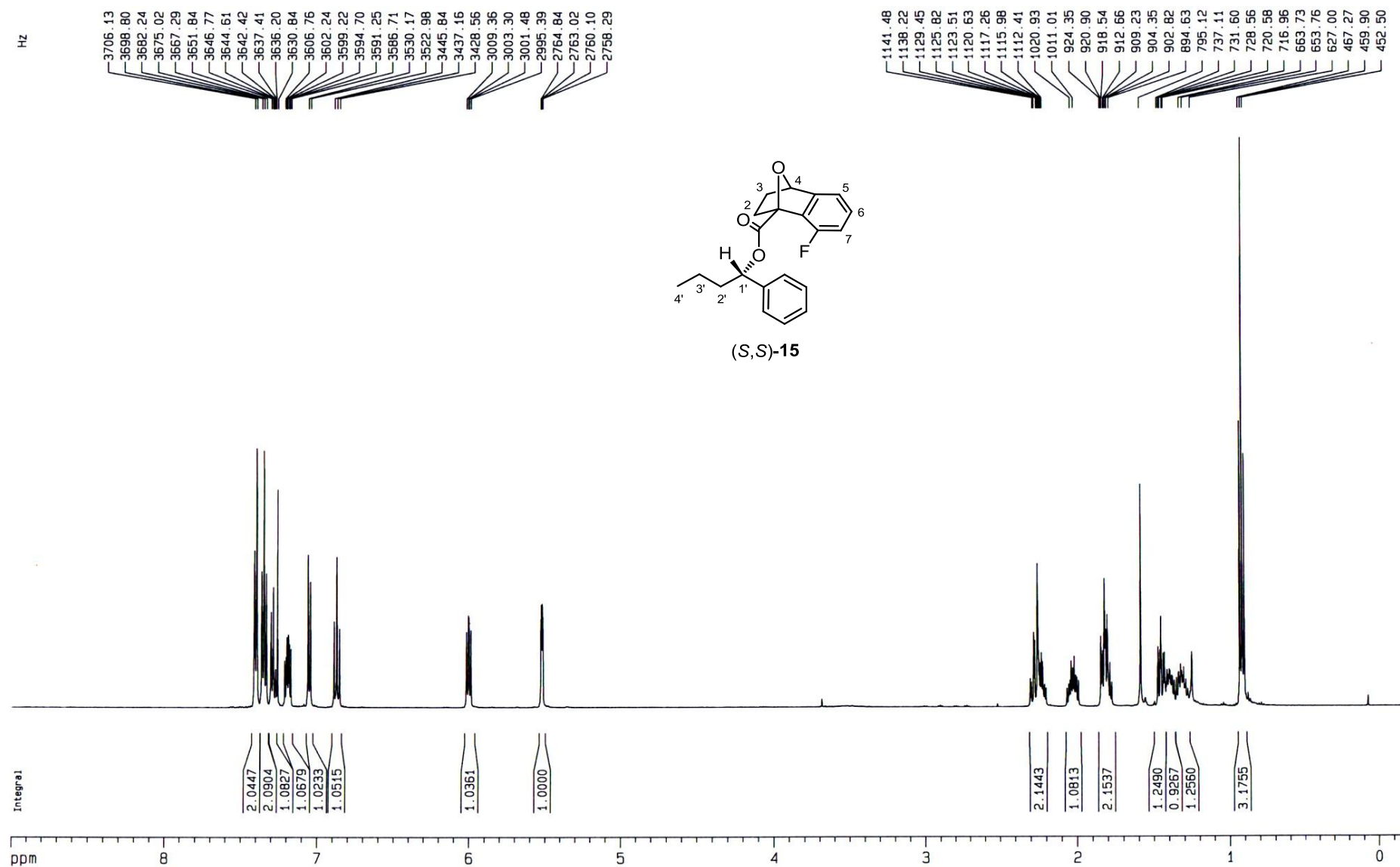


Figure 31. ¹H NMR spectrum of (1*S*,4*R*)-(*S*)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,S*)-15).

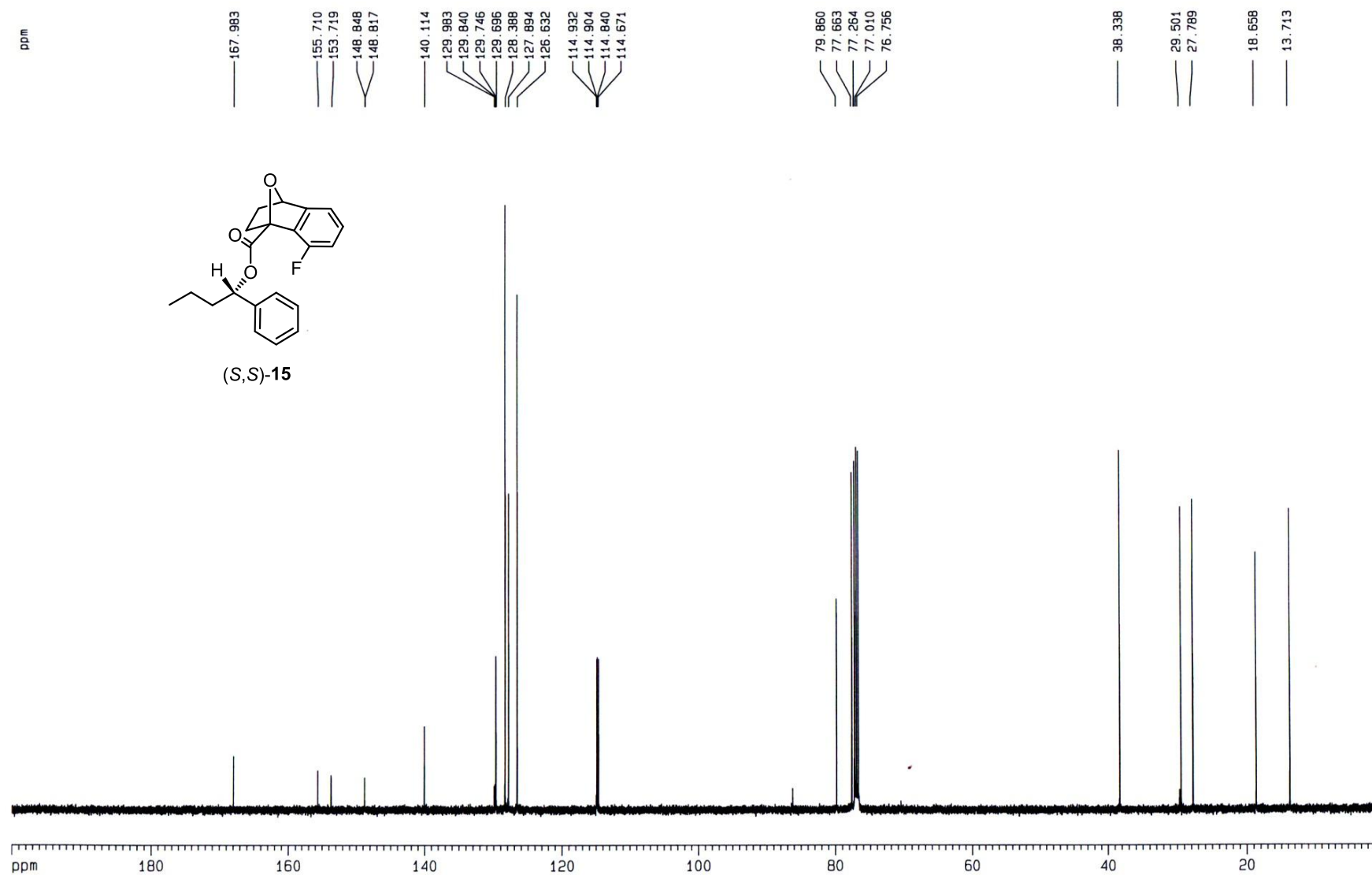


Figure 32. ¹³C NMR spectrum of (1*S*,4*R*)-(*S*)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate. ((*S,S*)-15)

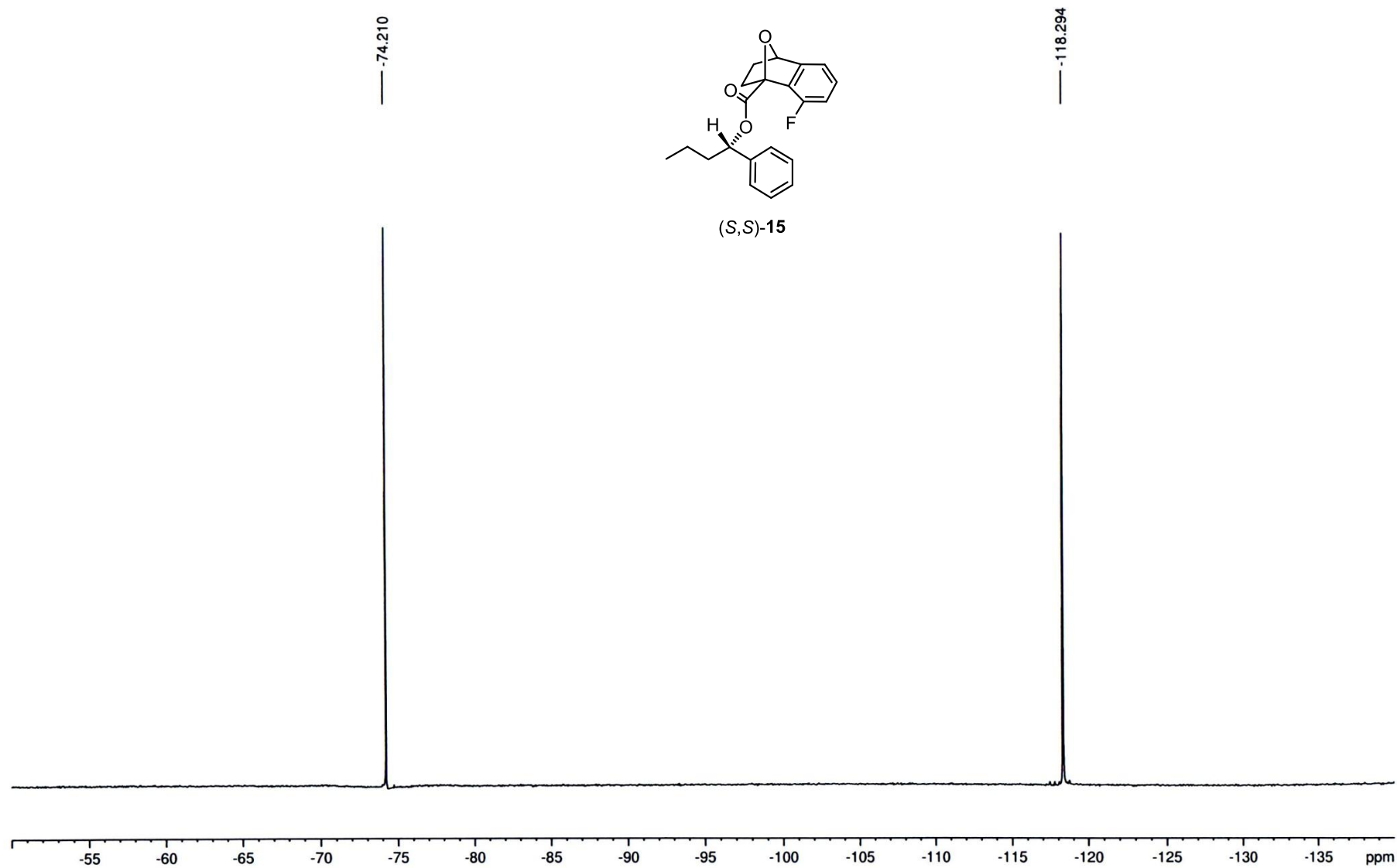


Figure 33. ^{19}F NMR spectrum of (1S,4R)-(S)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,S)-15).

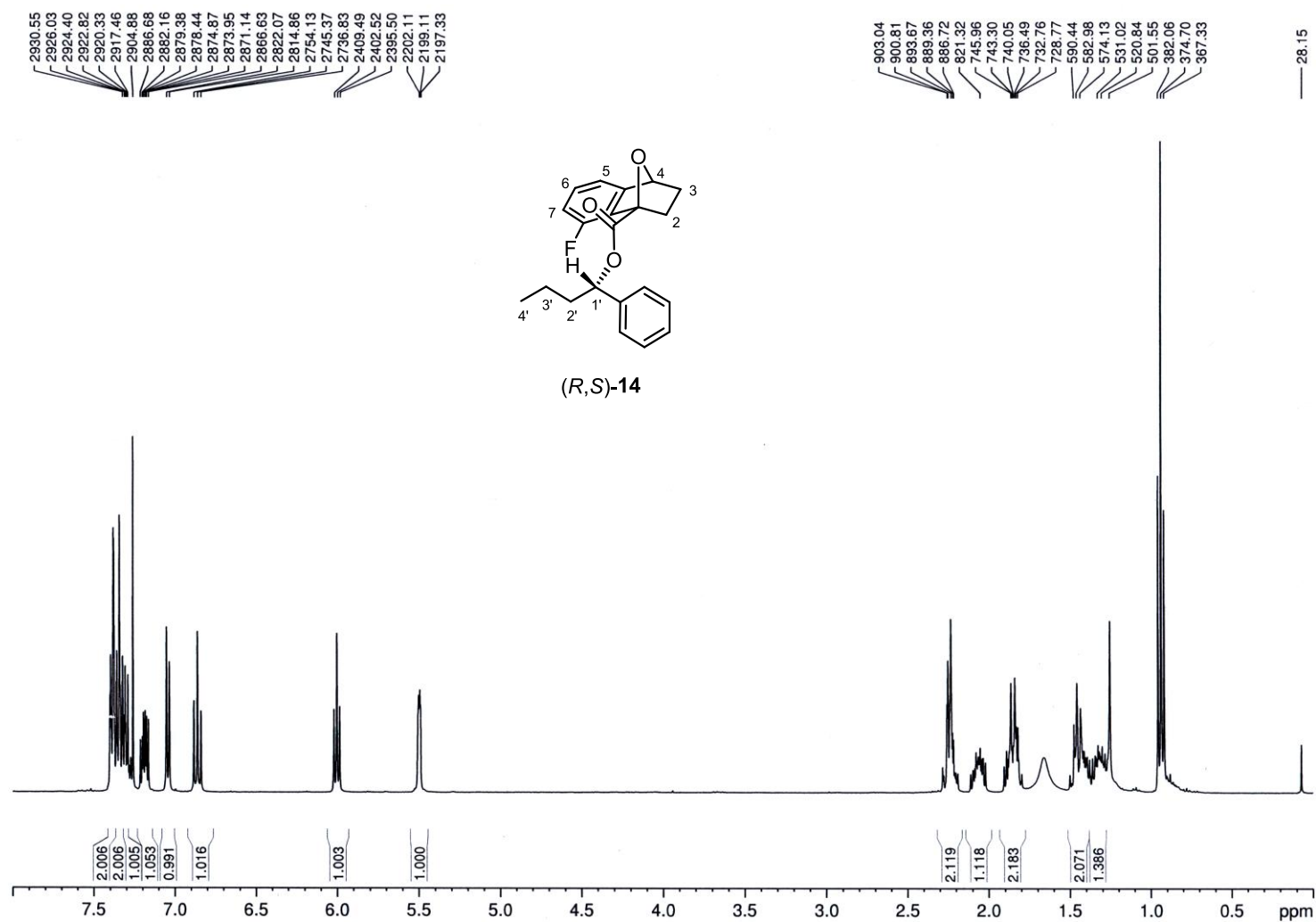


Figure 34. ^1H NMR spectrum of (1*R*,4*S*)-(S)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-14).

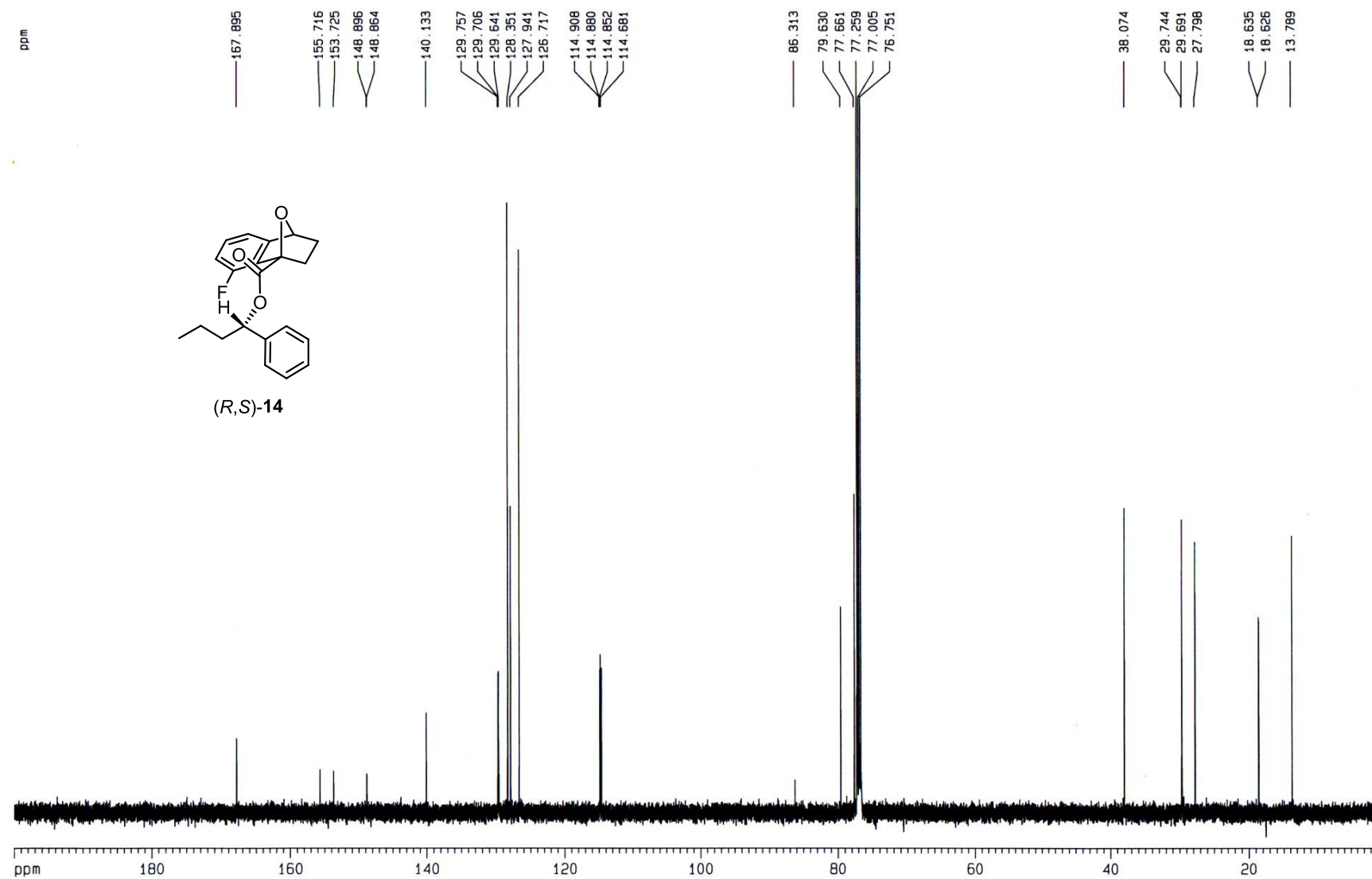


Figure 35. ¹³C NMR spectrum of (1*R*,4*S*)-(S)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-14).

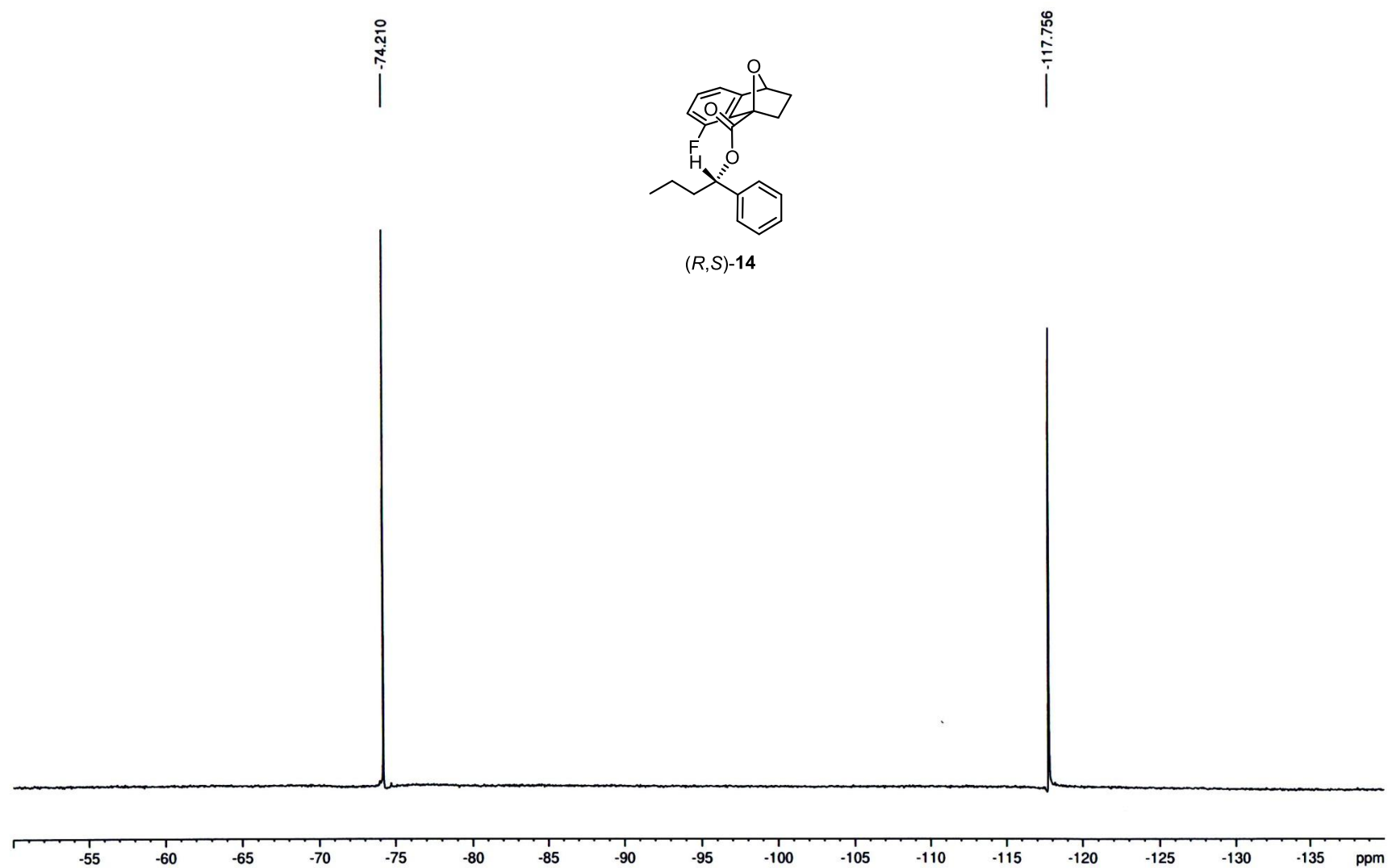


Figure 36. ¹H NMR spectrum of (1*R*,4*S*)-(S)-1-phenylbutyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R*,*S*)-**14**).

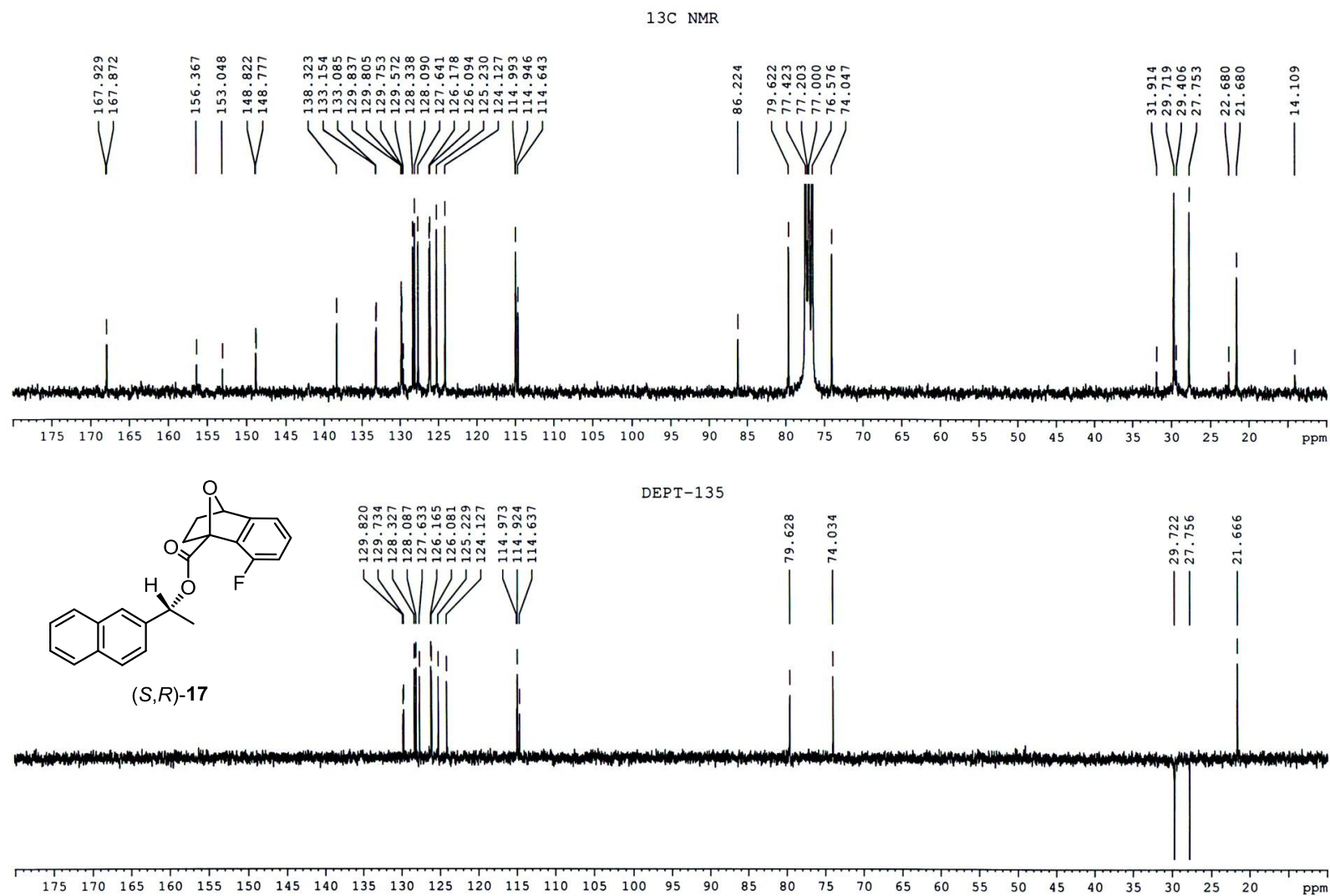


Figure 38. ^{13}C NMR spectra of (1*S*,4*R*)-(R)-1-(naphthalen-2-yl)ethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S*,*R*)-17).

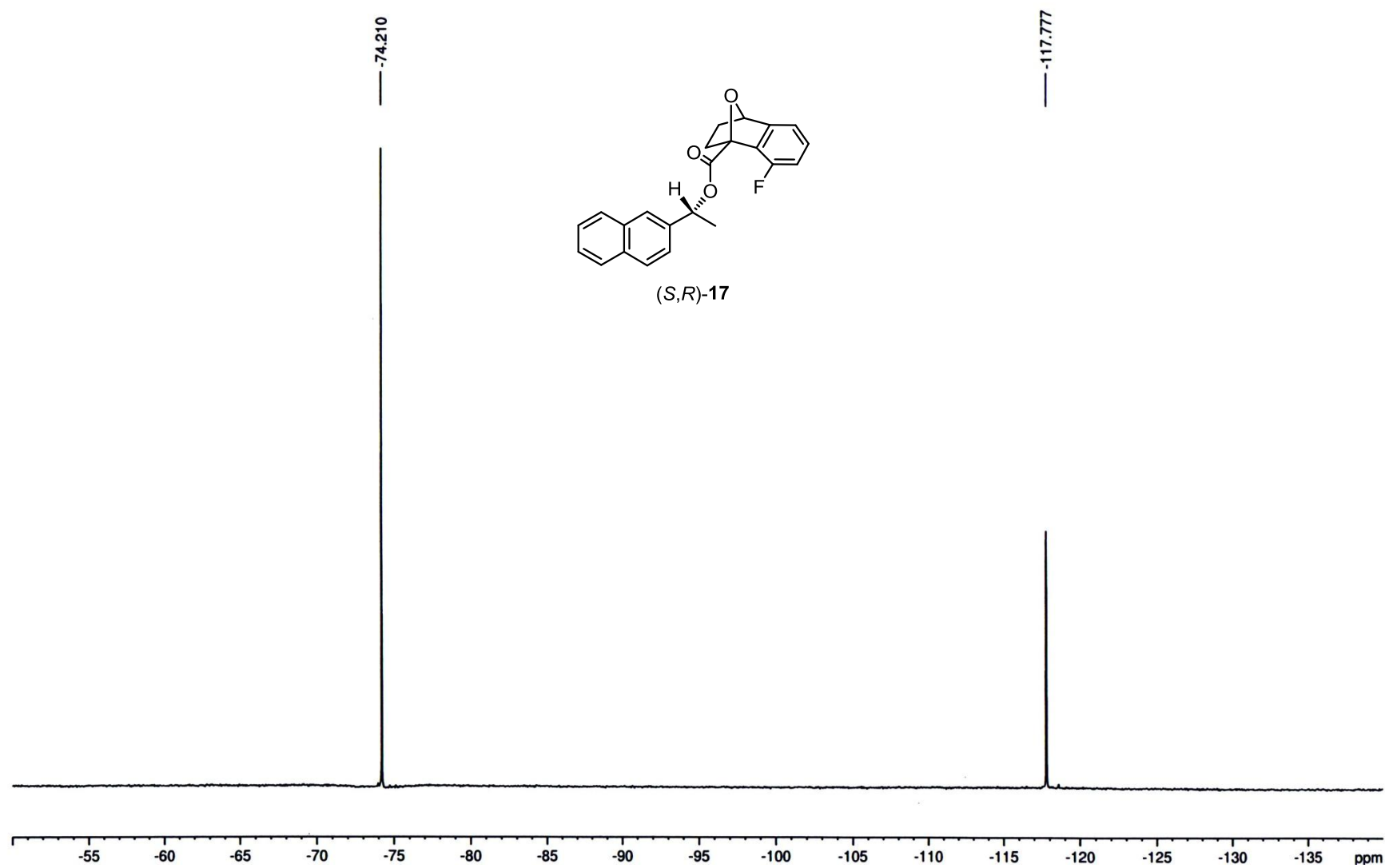


Figure 39. ^{19}F NMR spectrum of (1*S*,4*R*)-(*R*)-1-(naphthalen-2-yl)ethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,R*)-17).

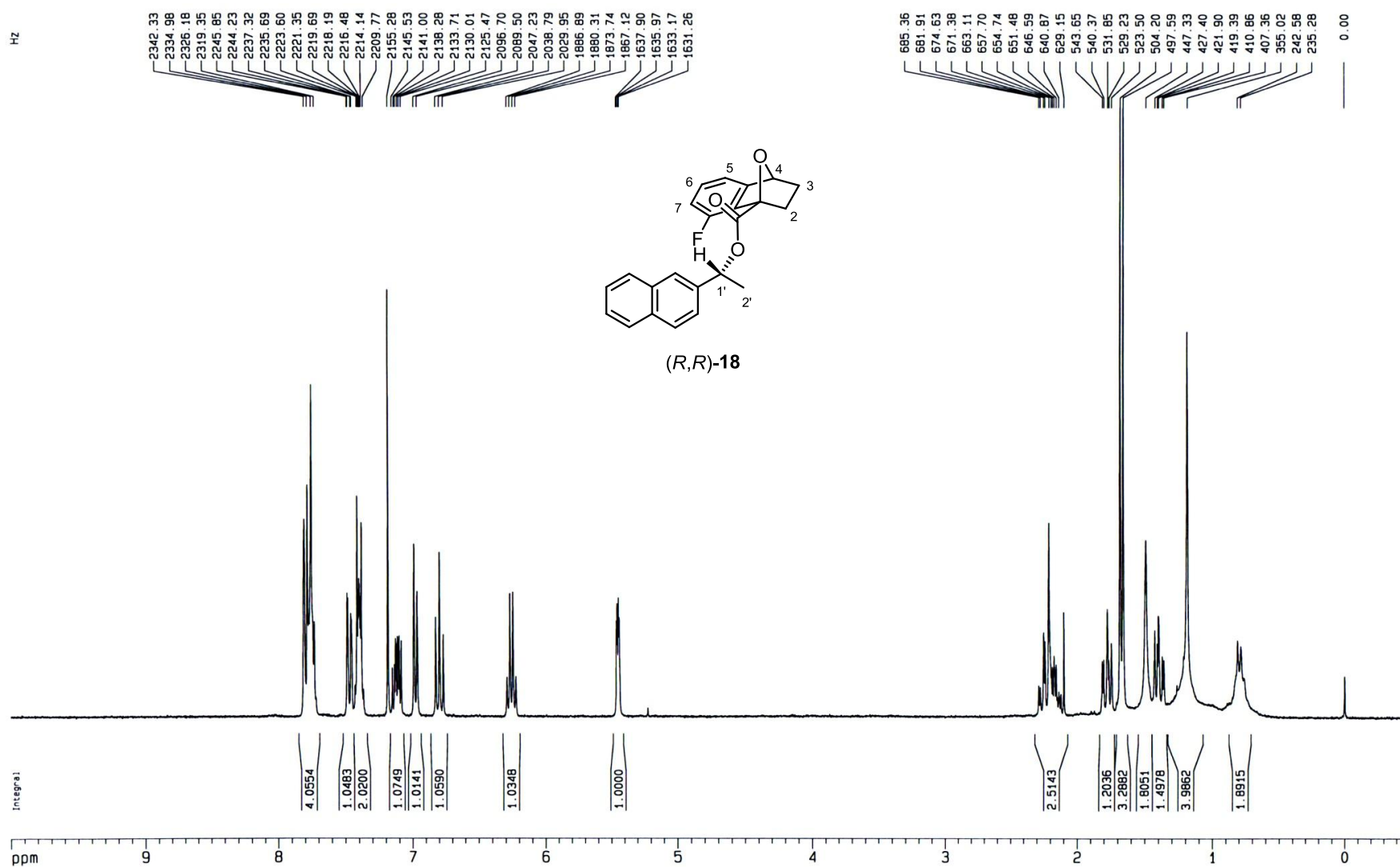


Figure 40. ¹H NMR spectrum of (1*R*,4*S*)-(*R*)-1-(naphthalen-2-yl)ethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,R*)-**18**).

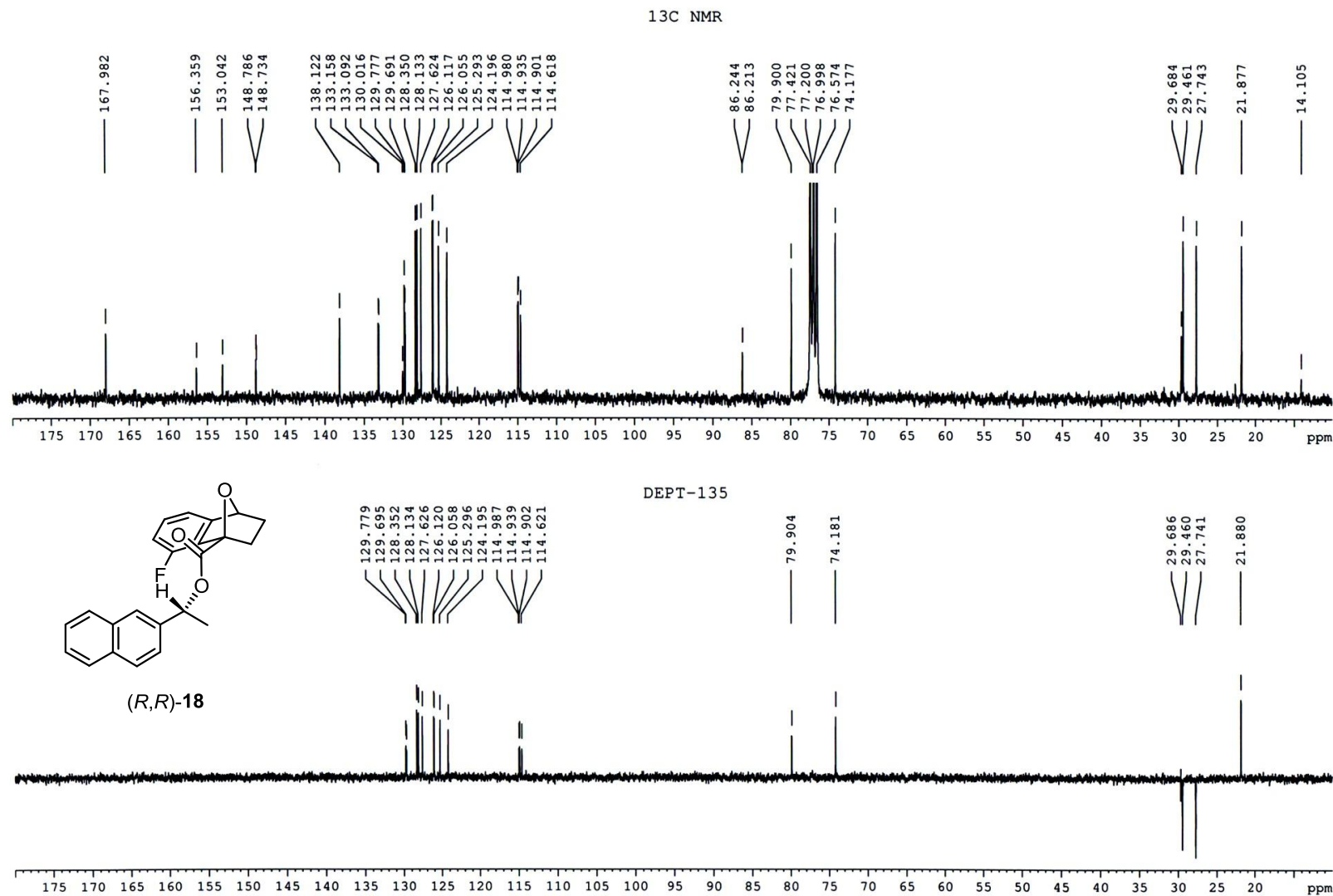


Figure 41. ¹³C NMR spectrum of (1R,4S)-(R)-1-(naphthalen-2-yl)ethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((R,R)-18).

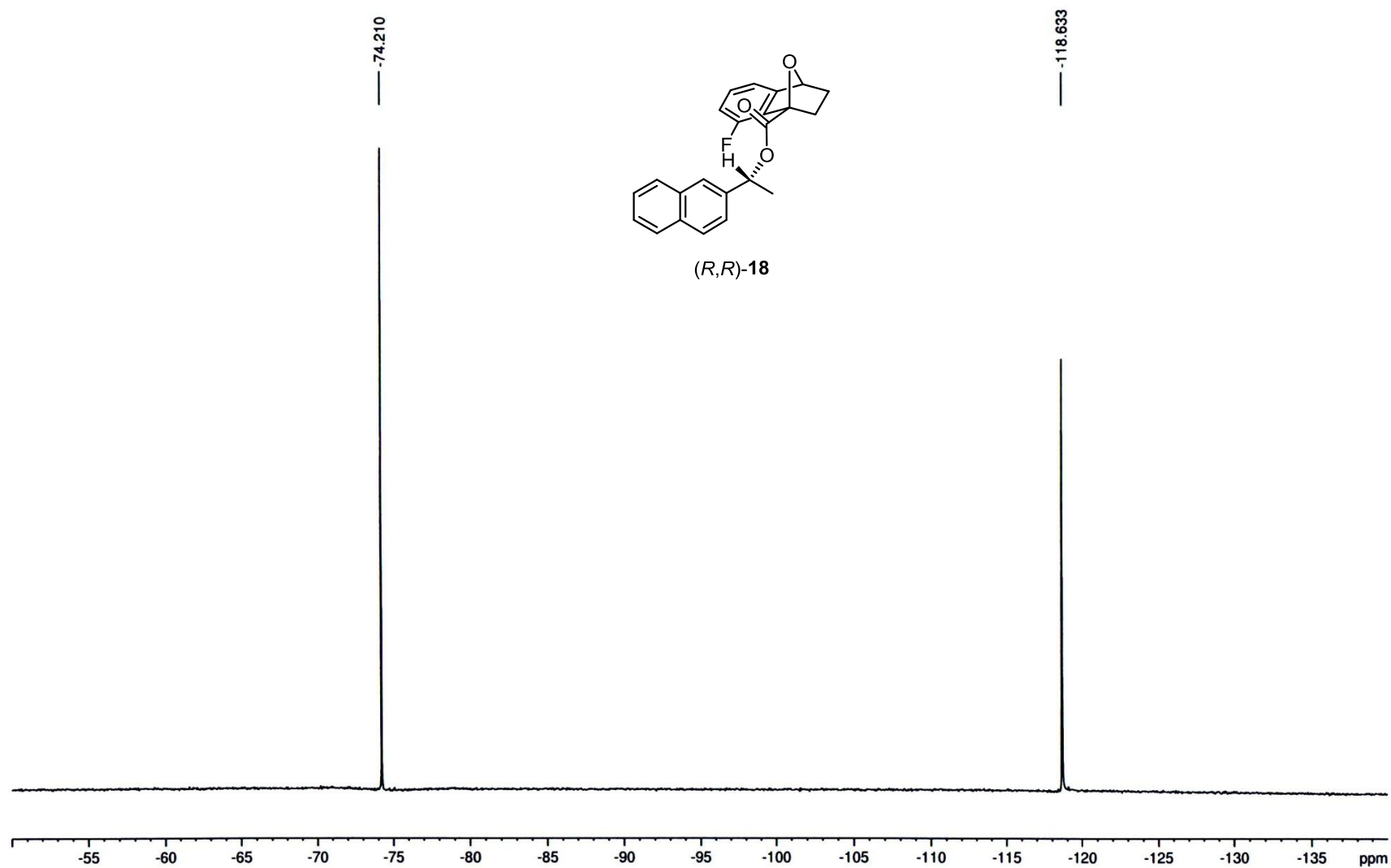


Figure 42. ^{19}F NMR spectrum of (1*R*,4*S*)-(R)-1-(naphthalen-2-yl)ethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,R*)-**18**).

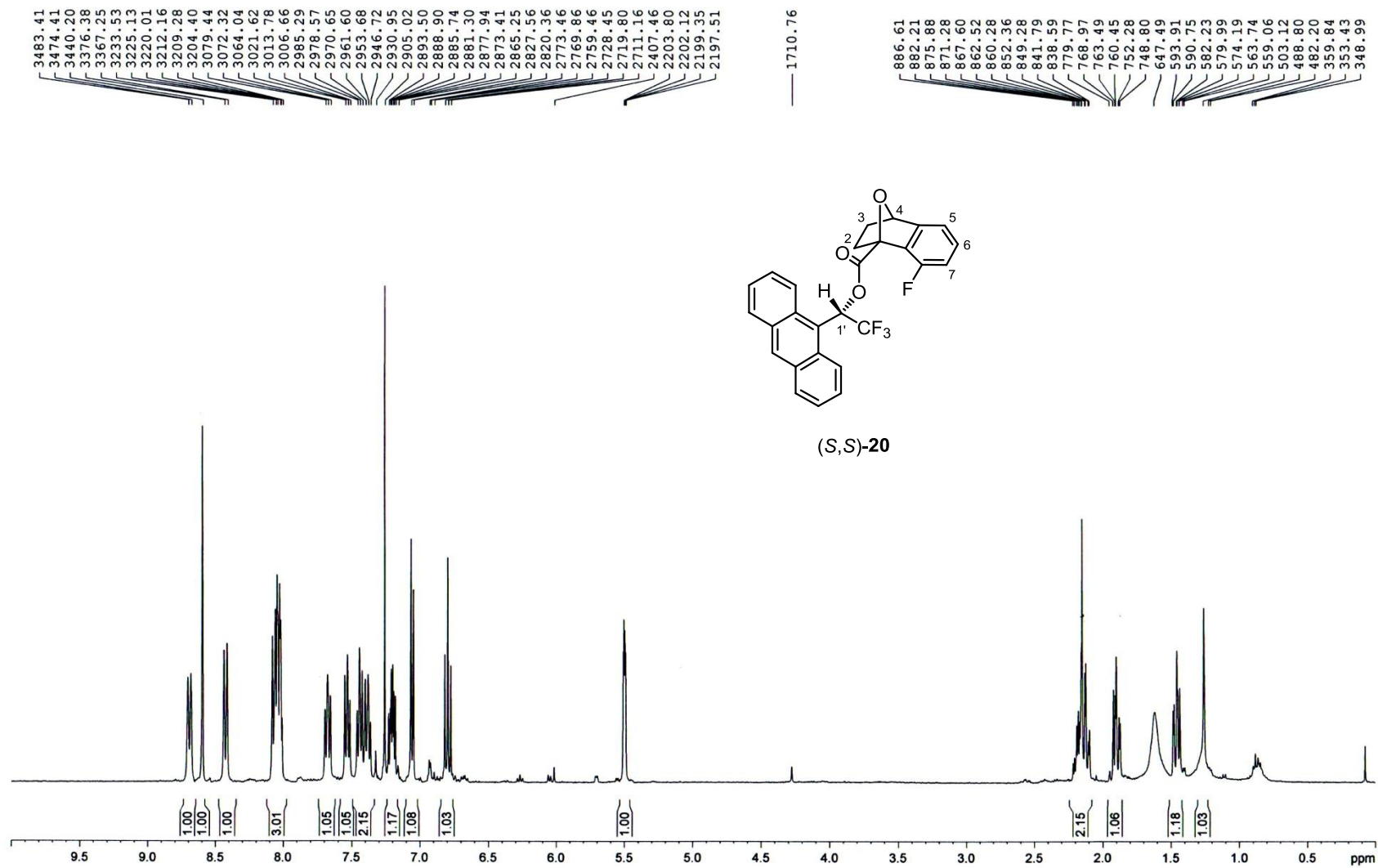


Figure 43. ¹H NMR spectrum of (1*S*,4*R*)-(*S*)-1-(anthracen-9-yl)-2,2,2-trifluoroethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,S*)-**20**).

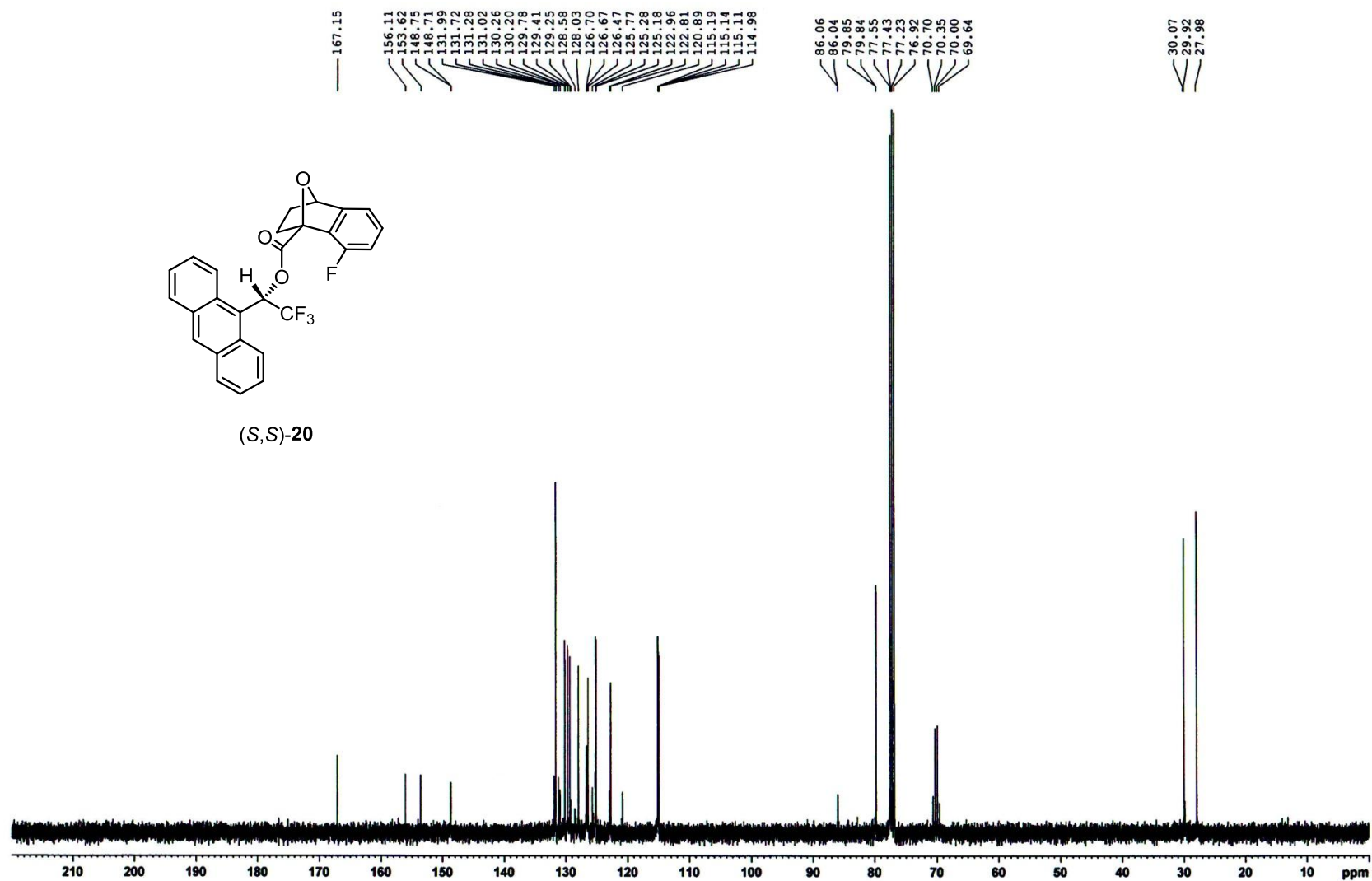


Figure 44. ¹³C NMR spectrum of (1*S*,4*R*)-(*S*)-1-(anthracen-9-yl)-2,2,2-trifluoroethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,S*)-**20**).

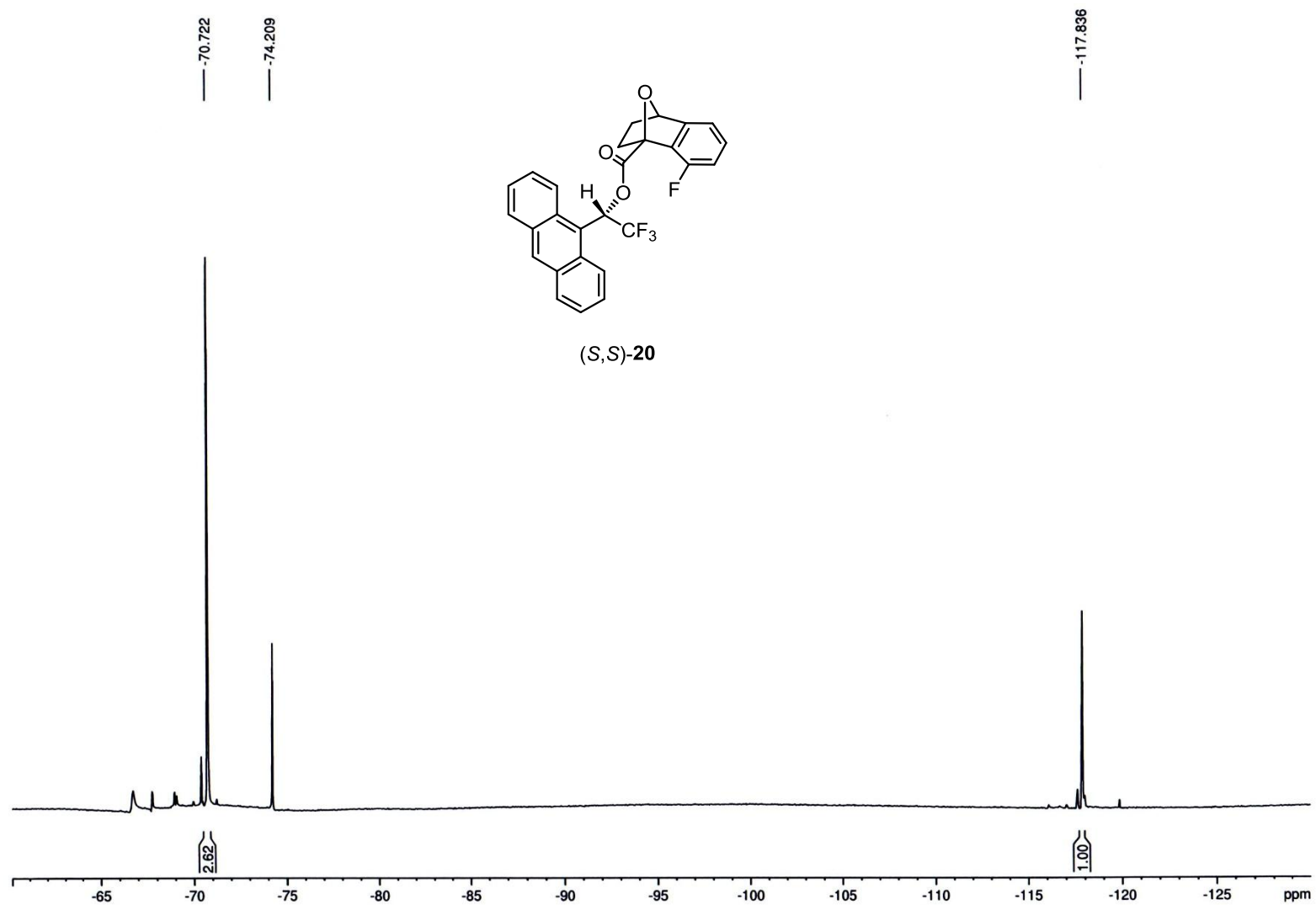


Figure 45. ¹⁹F NMR spectrum of (1S,4R)-(S)-1-(anthracen-9-yl)-2,2,2-trifluoroethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S,S)-20).

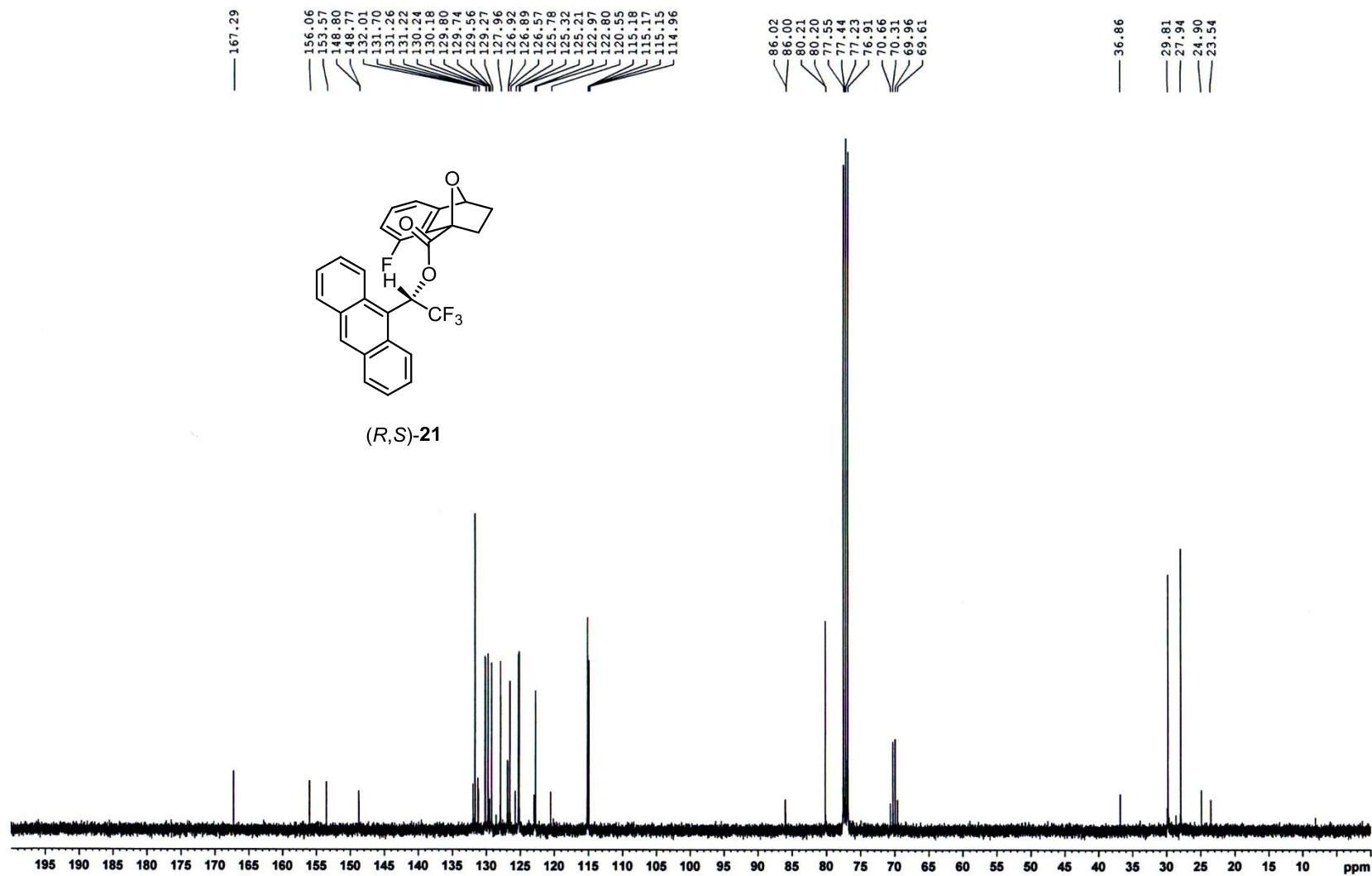


Figure 47. ¹³C NMR spectrum of (1*R*,4*S*)-(S)-1-(anthracen-9-yl)-2,2,2-trifluoroethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-21).

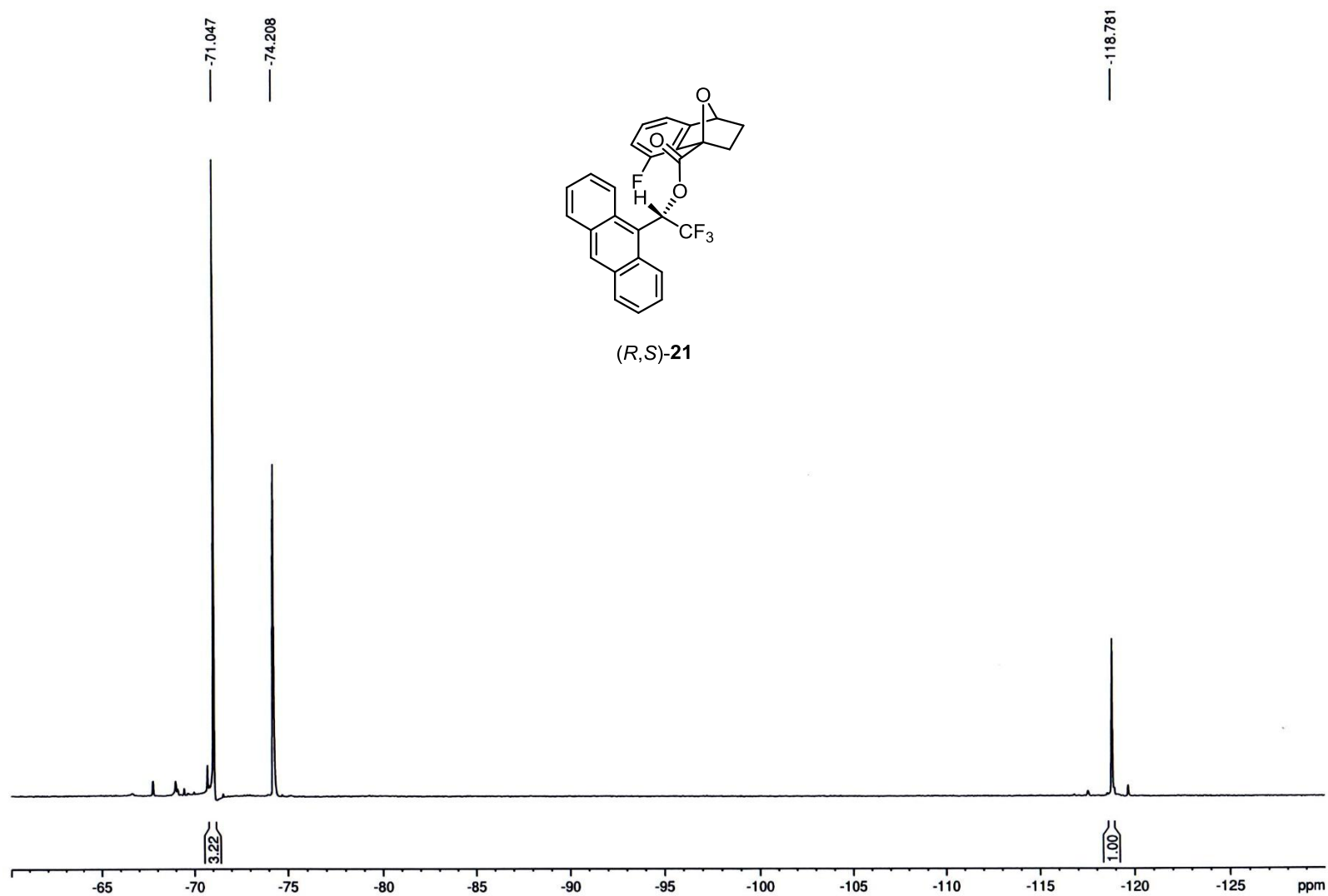


Figure 48. ^{19}F NMR spectrum of (1*R*,4*S*)-(S)-1-(anthracen-9-yl)-2,2,2-trifluoroethyl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-**21**).

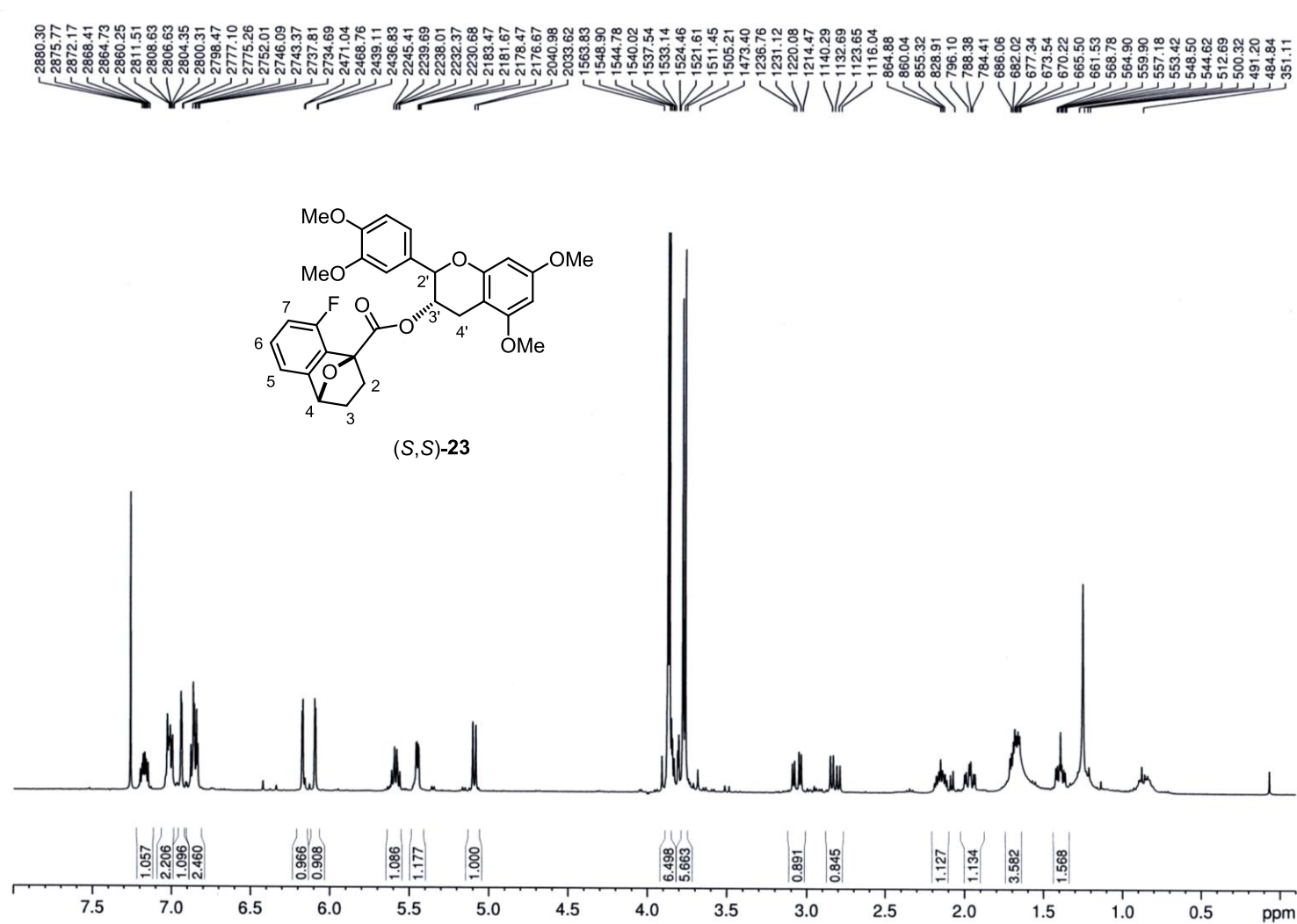


Figure 49. ^1H NMR spectrum of (1*S*,4*R*)-(3*S*)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-yl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,S*)-23).

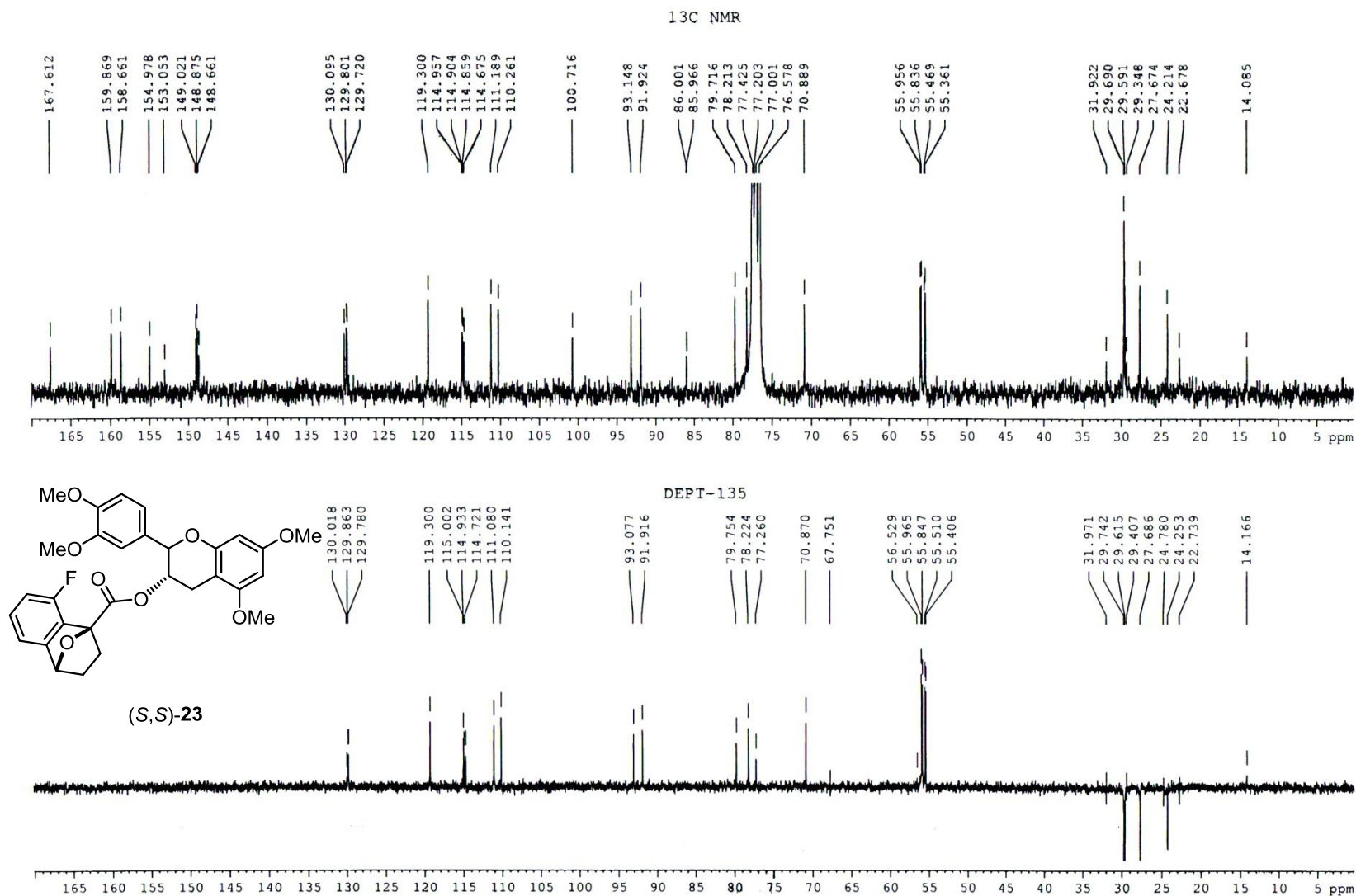


Figure 50. ^{13}C NMR spectra of (1*S*,4*R*)-(3*S*)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-yl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,S*)-23).

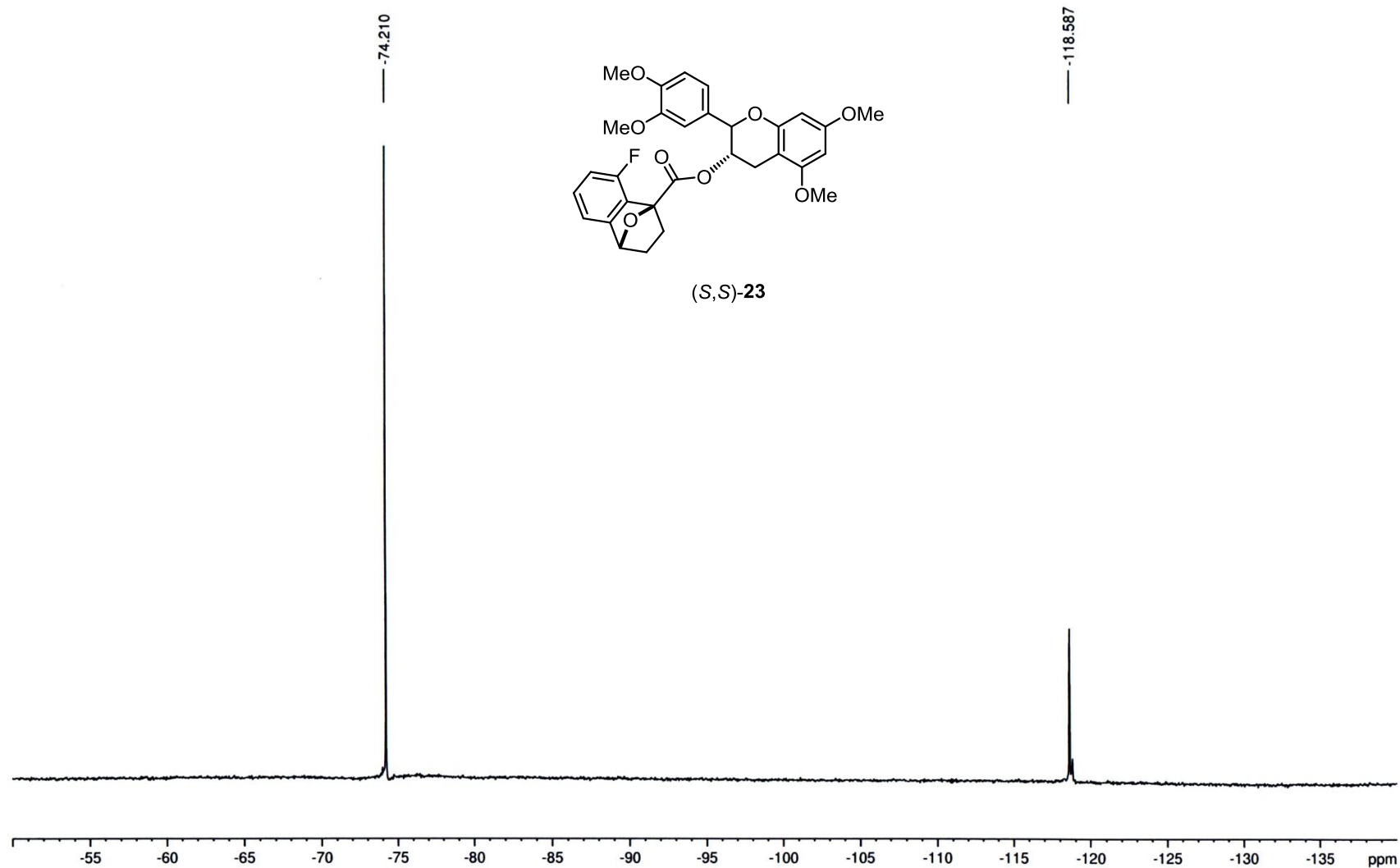


Figure 51. ^{19}F NMR spectrum of (1*S*,4*R*)-(3*S*)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-yl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*S,S*)-**23**).

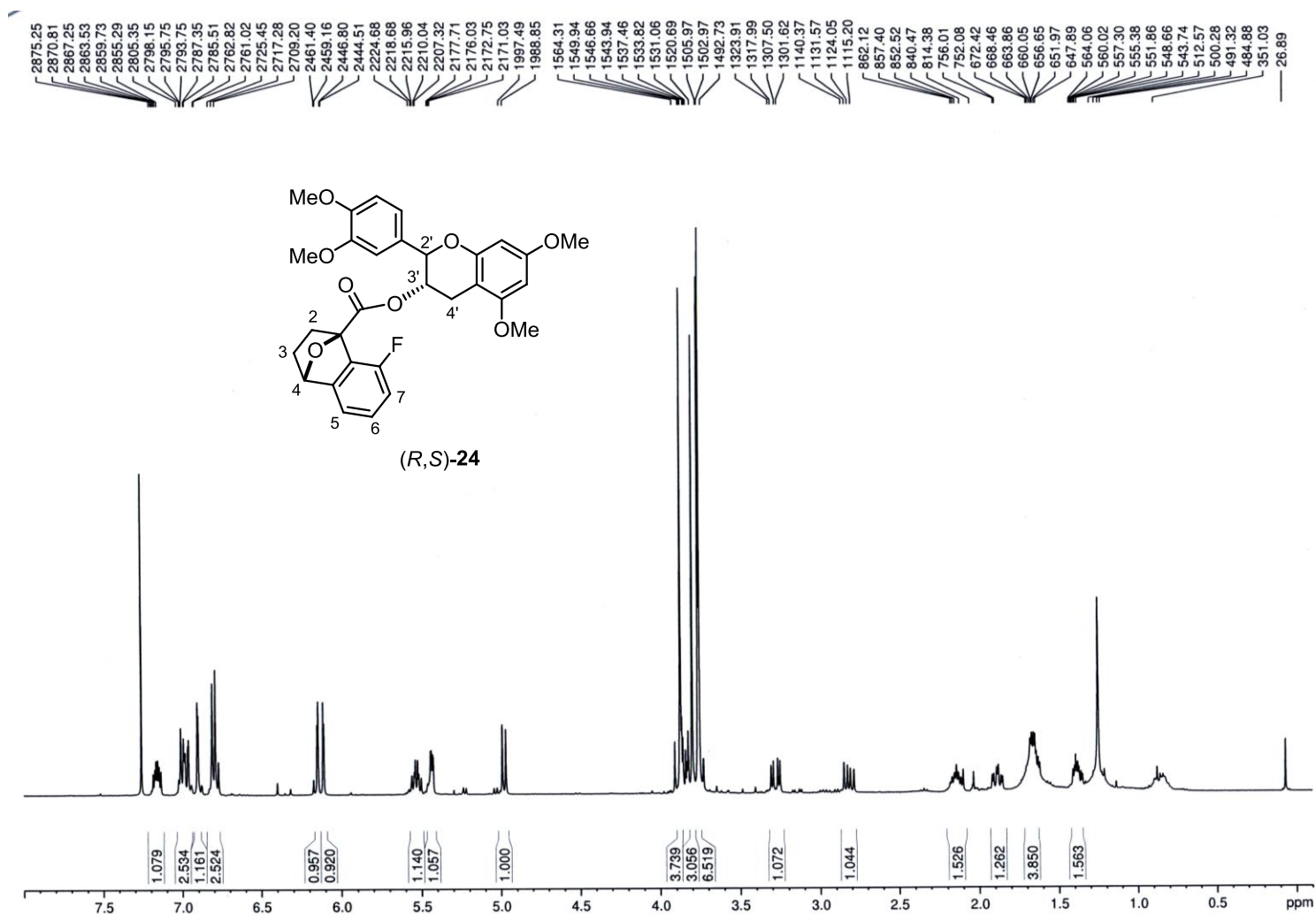


Figure 52. ¹H NMR spectrum of (1*R*,4*S*)-(3*S*)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-yl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-24).

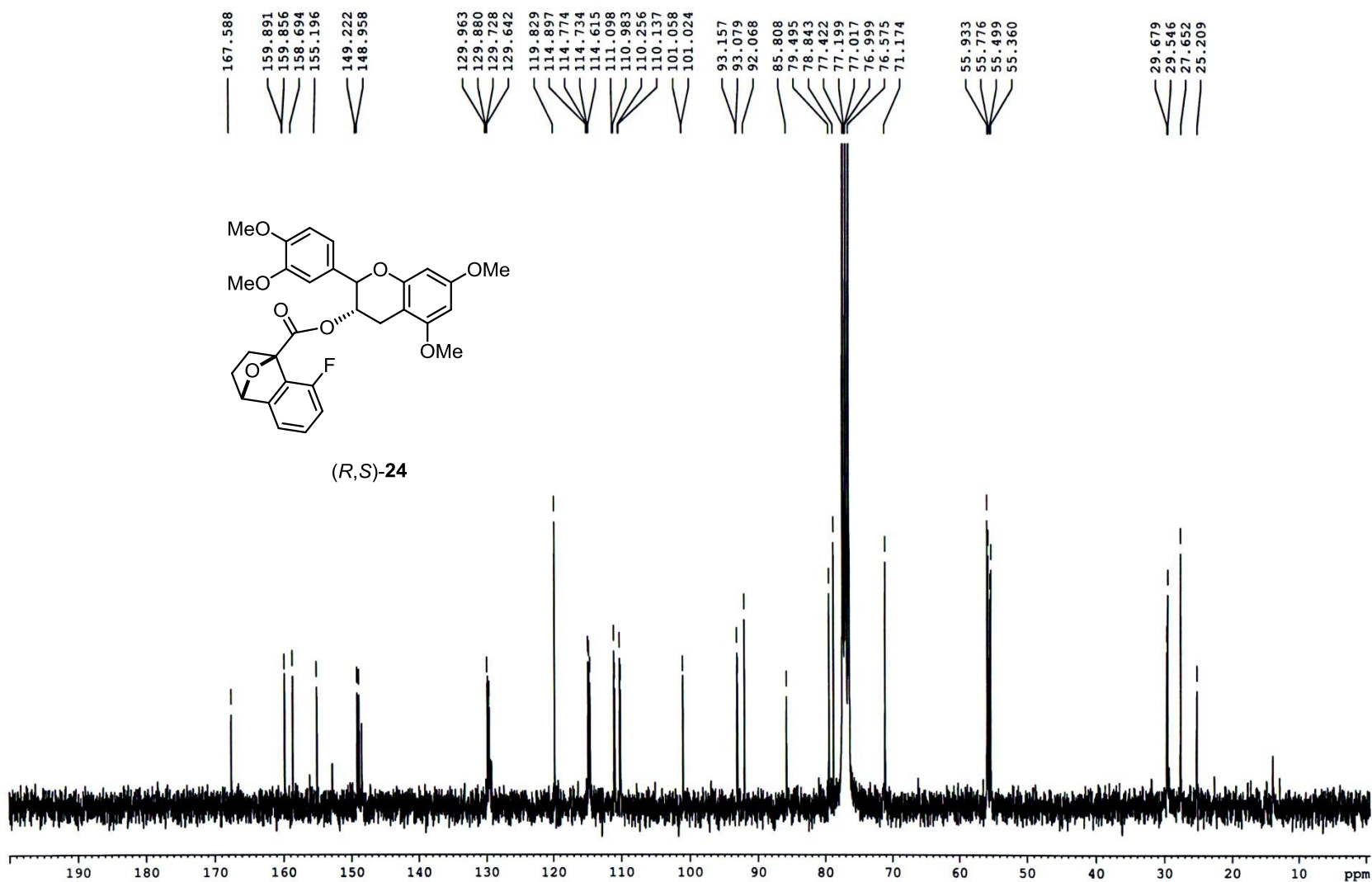


Figure 53. ^{13}C NMR spectrum of (1*R*,4*S*)-(3*S*)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-yl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-24).

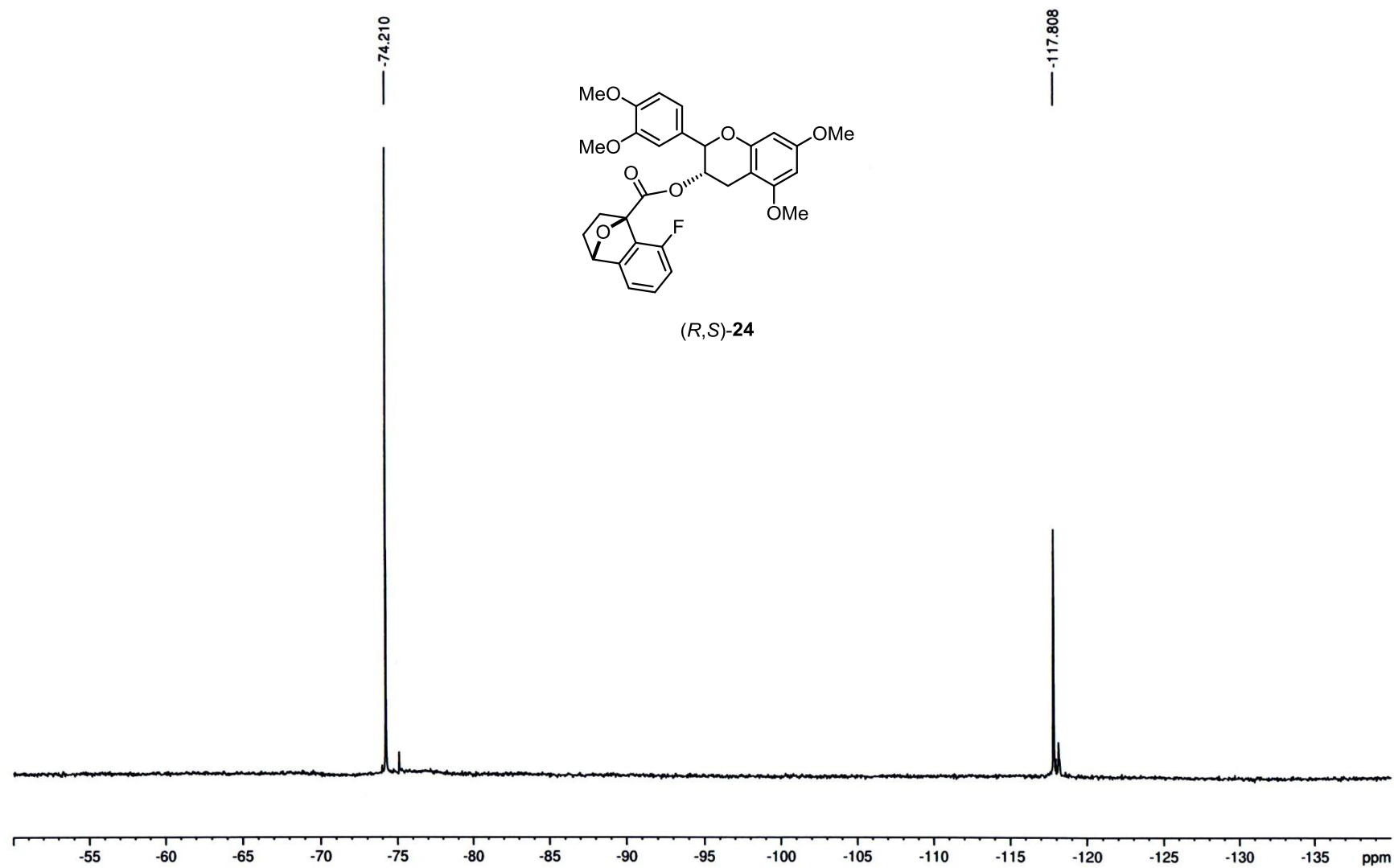
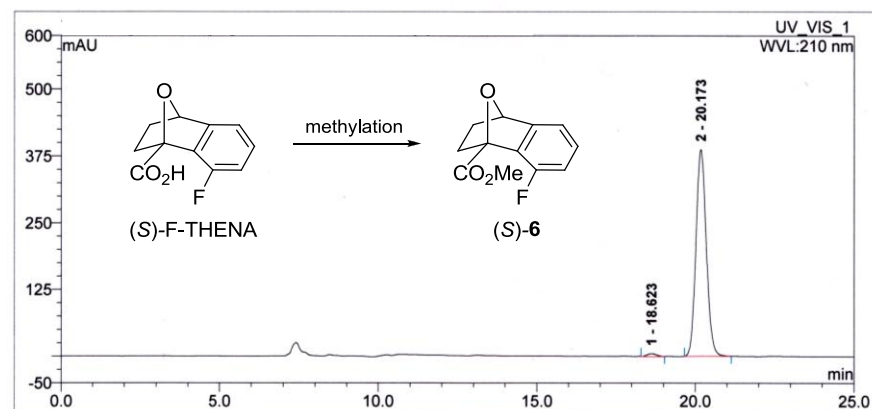
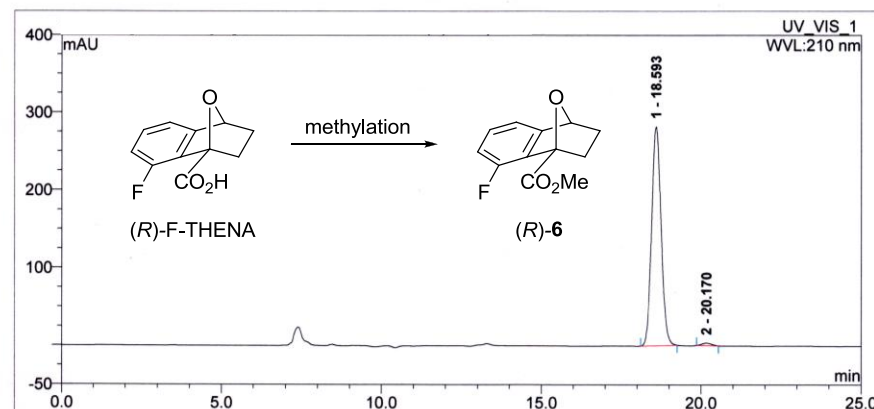


Figure 54. ^{19}F NMR spectrum of (1*R*,4*S*)-(3*S*)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-yl 8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((*R,S*)-**24**).



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.62	na	4.887	1.596	1.08	n.a.	BMB*
2	20.17	na	387.000	145.996	98.92	n.a.	BMB*
Total:			391.886	147.591	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.59	na	281.915	97.031	98.87	n.a.	BMB*
2	20.17	na	3.215	1.106	1.13	n.a.	BMB*
Total:			285.130	98.138	100.00	0.000	

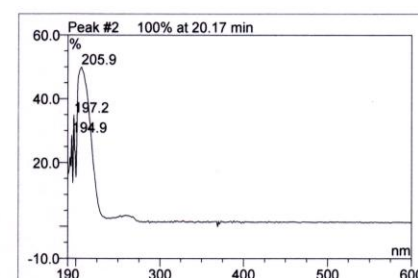
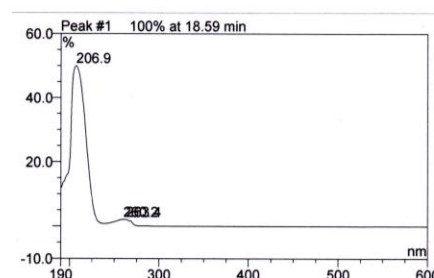
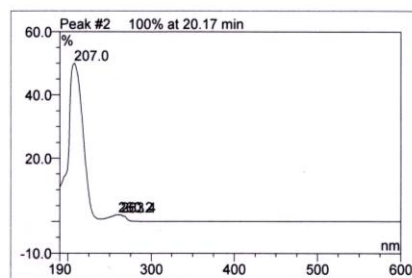
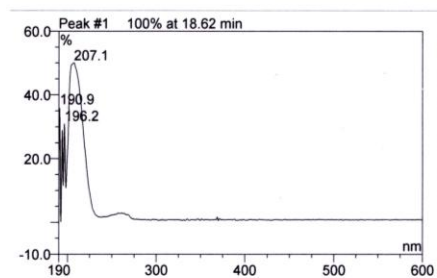


Figure 55. HPLC chromatograms of methyl (S)-8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((S)-6) and methyl (R)-8-fluoro-1,2,3,4-tetrahydro-1,4-epoxynaphthalene-1-carboxylate ((R)-6).