

SUPPORTING INFORMATION

Synthesis of Sugar Diene and its Pd-Catalyzed Transformation into Chromanes

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Crystal Data:

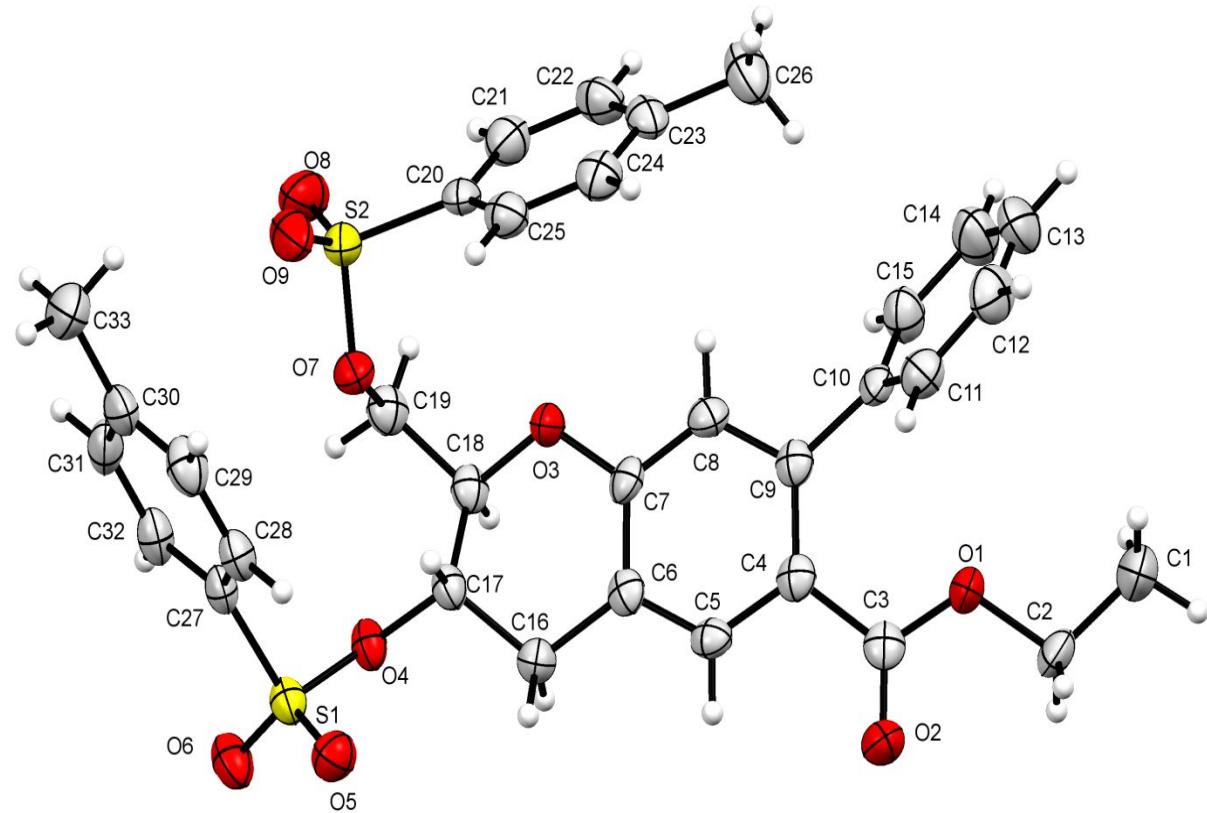


Figure S1. Thermal ellipsoid diagram for compound 7 with thermal ellipsoids shown at 50% probability level

X-Ray diffraction studies on (2*R*,3*S*)-2-tosyloxymethyl-3-tosyloxy-6-ethoxycarbonyl-7-phenylchromane (7)

Single crystal for X-ray diffraction studies were grown by dissolving the compound **7** in a mixture of ethyl acetate and petroleum ether and allowing slow evaporation of the solvent at room temperature. The X-ray diffraction data was collected at temperature 100 K with graphite monochromated Mo/K α radiation ($\lambda = 0.71073 \text{ \AA}$). The structure was solved by direct methods using SHELXS-97 and then refined by full-matrix least-squares method on F2 (SHELXL-97).¹ All calculations were carried out using WinGX package of the crystallographic programs.² For molecular graphics, the program Mercury³ have been used. Molecular structure was drawn using ORTEP software as given in **Figure S1**. The complete crystallographic data has been given in **Table S1**.

Table S1. Single X-ray crystal data and structure refinement for compound **7**

Empirical formula	$C_{33}H_{32}O_9S_2$		
Formula weight	636.70		
Temperature	100 K		
Wavelength	0.71073 \AA		
Crystal system	Monoclinic		
Space group	C2		
Unit cell dimensions	$a = 33.185(5) \text{ \AA}$	$\alpha = 90^\circ$	
	$b = 5.9809(9) \text{ \AA}$	$\beta = 109.647 (3)^\circ$	
	$c = 16.116(3) \text{ \AA}$	$\gamma = 90^\circ$	
Volume	$3012.5(8) \text{ \AA}^3$		
Z	4		
Density (calculated)	1.404 mg/m ³		
Absorption coefficient	0.233 mm^{-1}		
F (000)	1336		
Crystal size	$0.2 \times 0.3 \times 0.2 \text{ mm}^3$		
Theta range for data collection	2.162 to 25.186°		
Index ranges	$-39 \leq h \leq 39, -7 \leq k \leq 7, -19 \leq l \leq 19$		
Reflections collected	18011		
Independent reflections	5366 [R(int) = 0.0676]		
Completeness to theta = 25.00°	99.1%		
Absorption correction	multi-scan		

Max. and min. transmission 0.954 and 0.946
Refinement method least-squares method
Data / restraints / parameters 5366/1/400
Goodness-of-fit on F^2 0.991
CCDC No. **1918104**

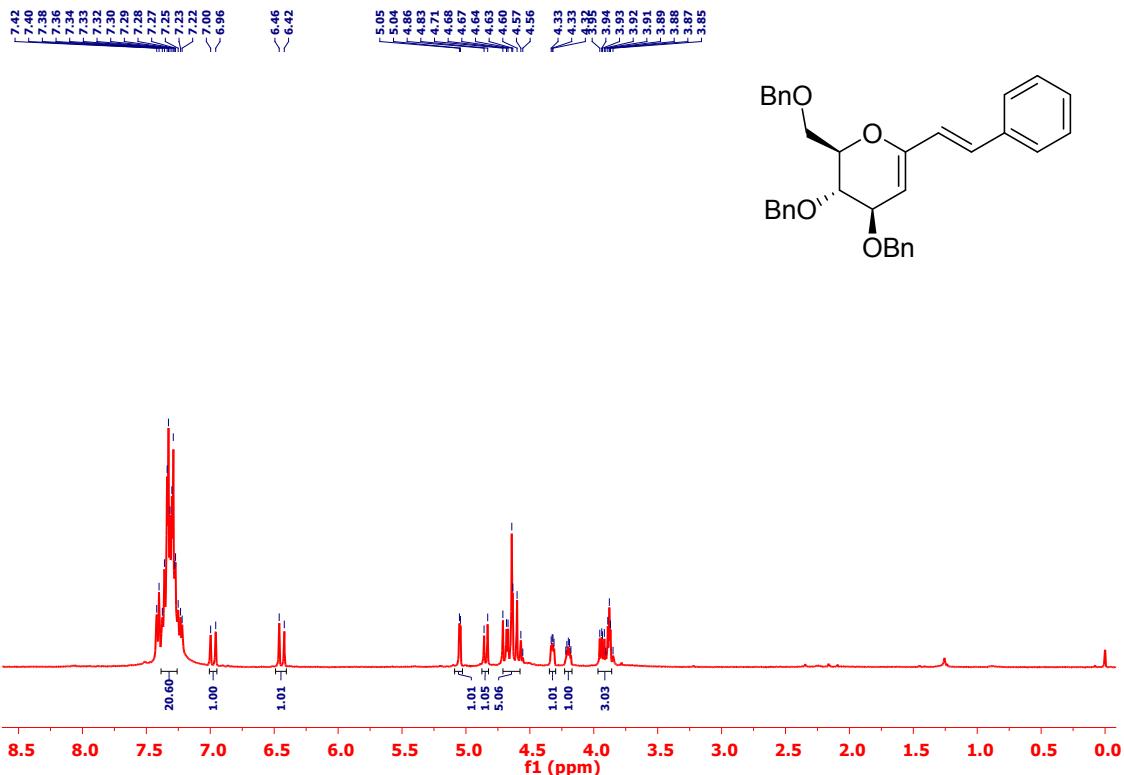


Figure S2. ¹H NMR spectrum of compound 2 (400 MHz, CDCl₃)

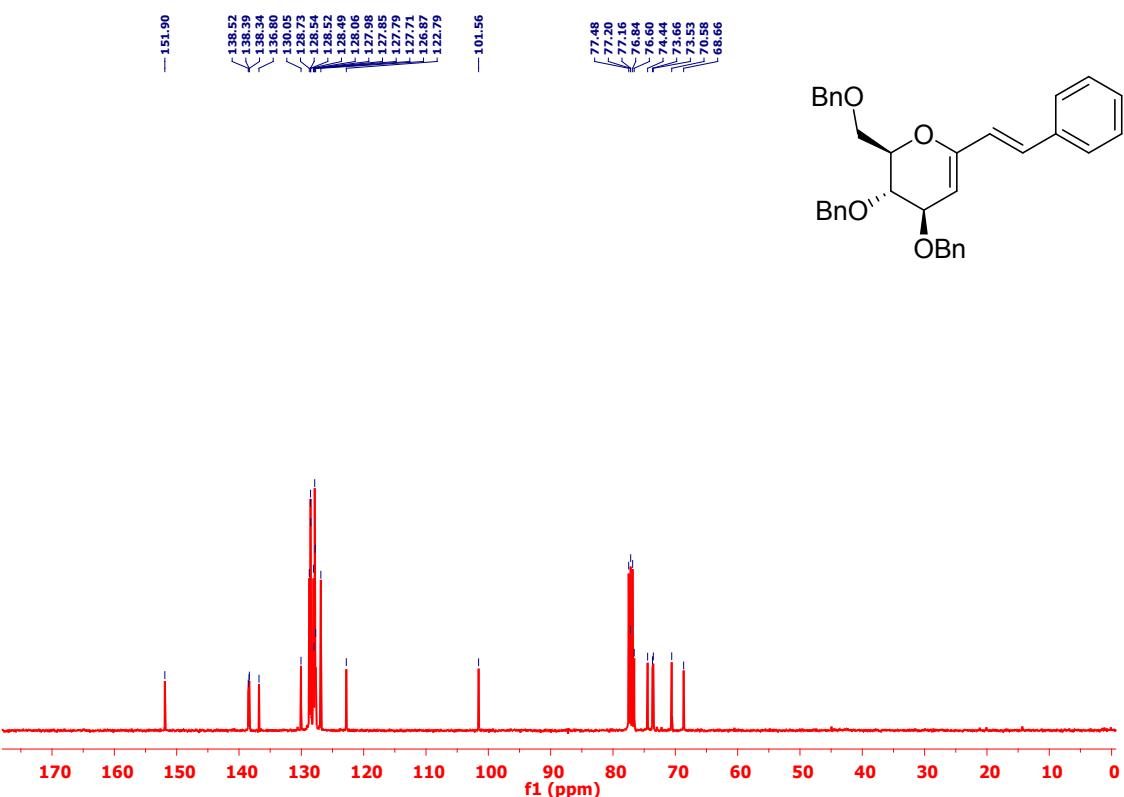


Figure S3. ¹³C NMR spectrum of compound 2 (100.6 MHz, CDCl₃)

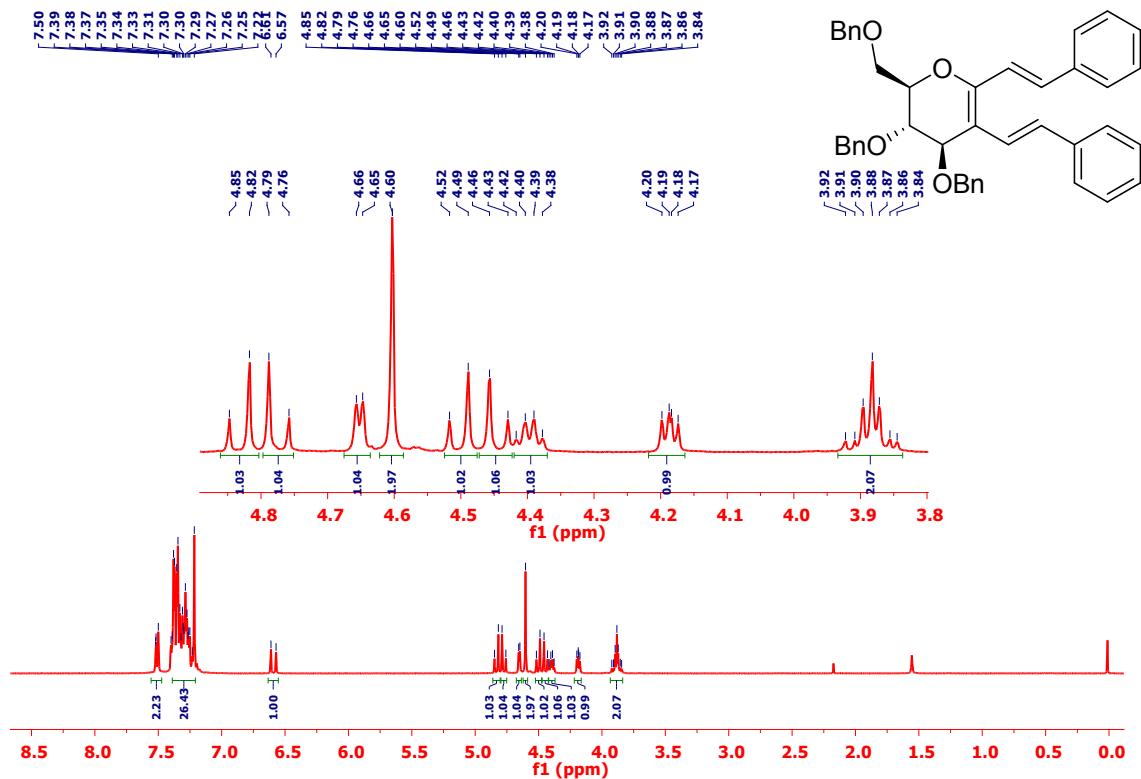


Figure S4. ¹H NMR spectrum of compound 4a (400 MHz, CDCl₃)

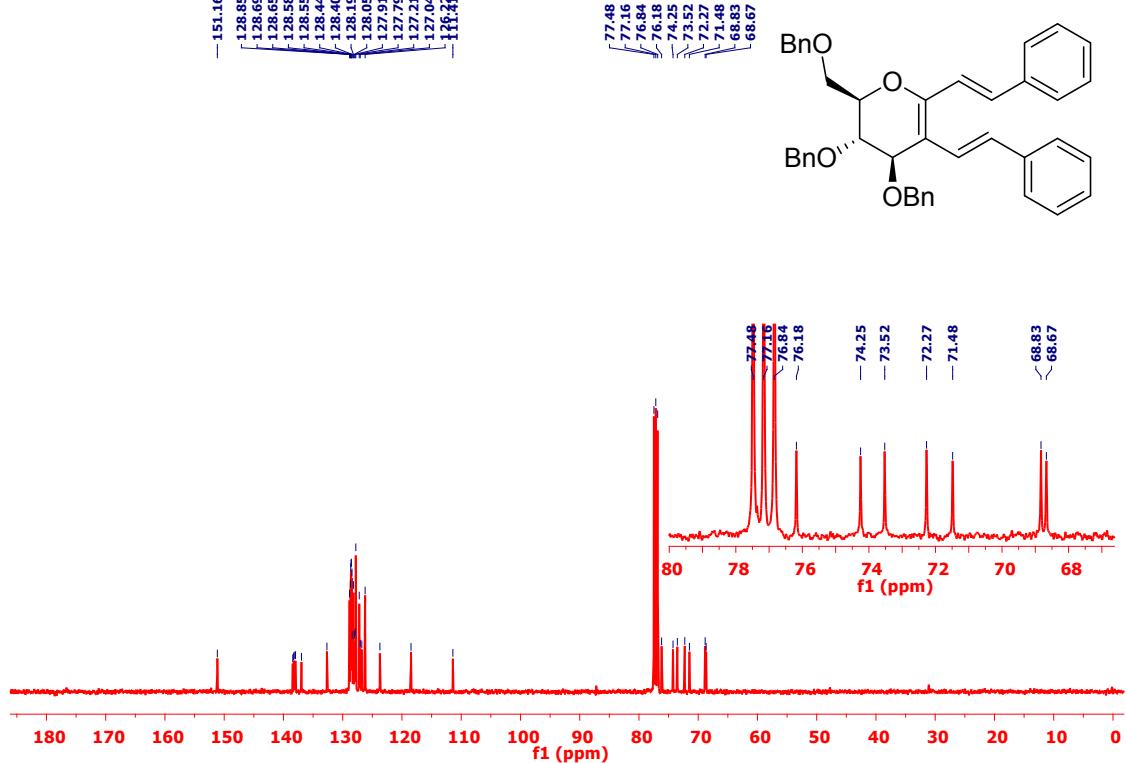


Figure S5. ¹³C NMR spectrum of compound 4a (100.6 MHz, CDCl₃)

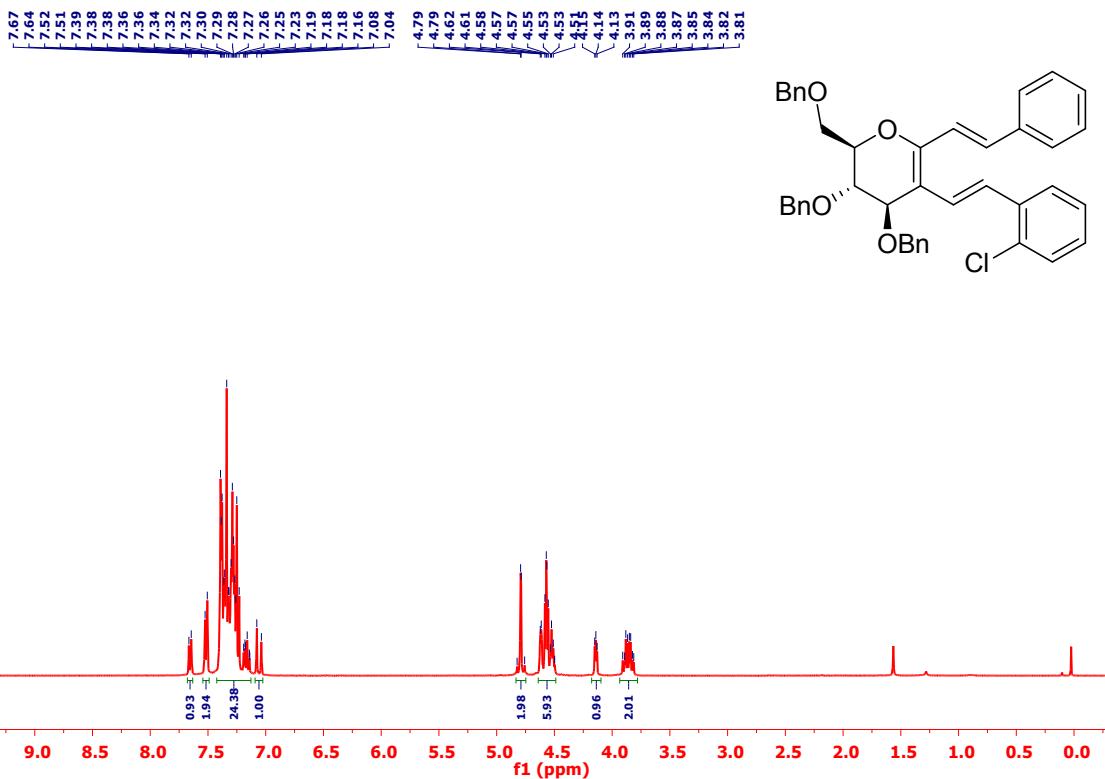


Figure S6. ¹H NMR spectrum of compound **4b** (400 MHz, CDCl₃)

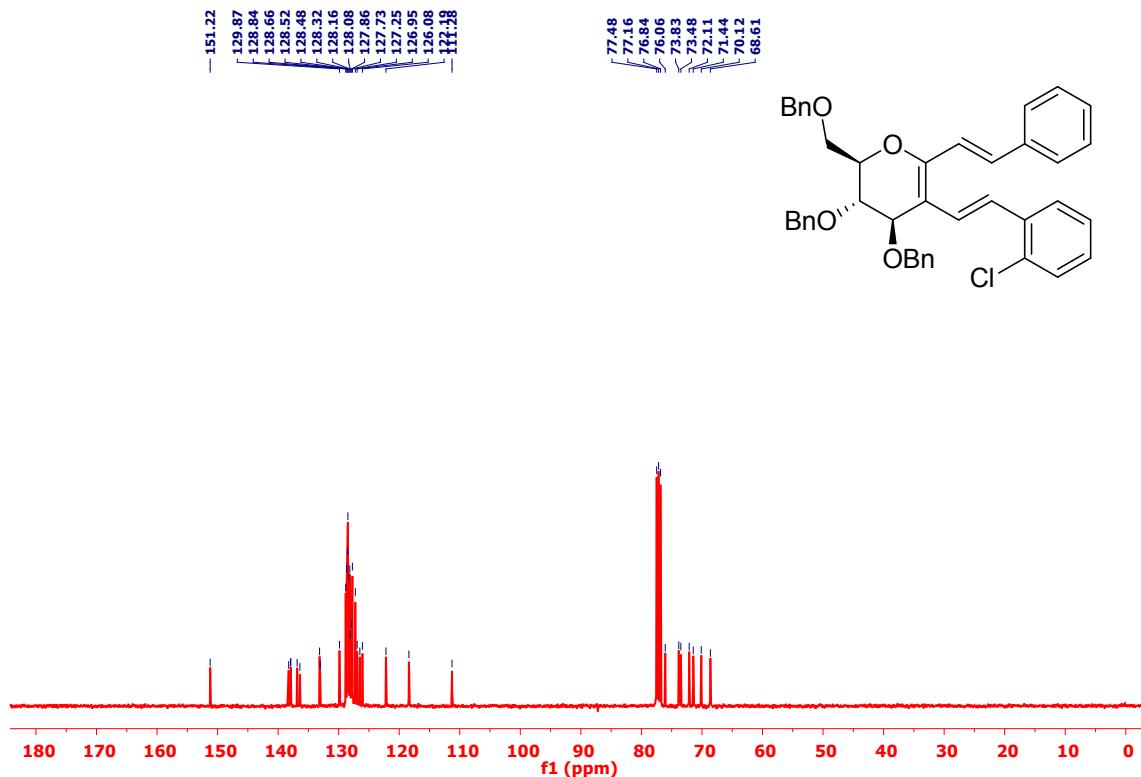


Figure S7. ¹³C NMR spectrum of compound **4b** (100.6 MHz, CDCl₃)

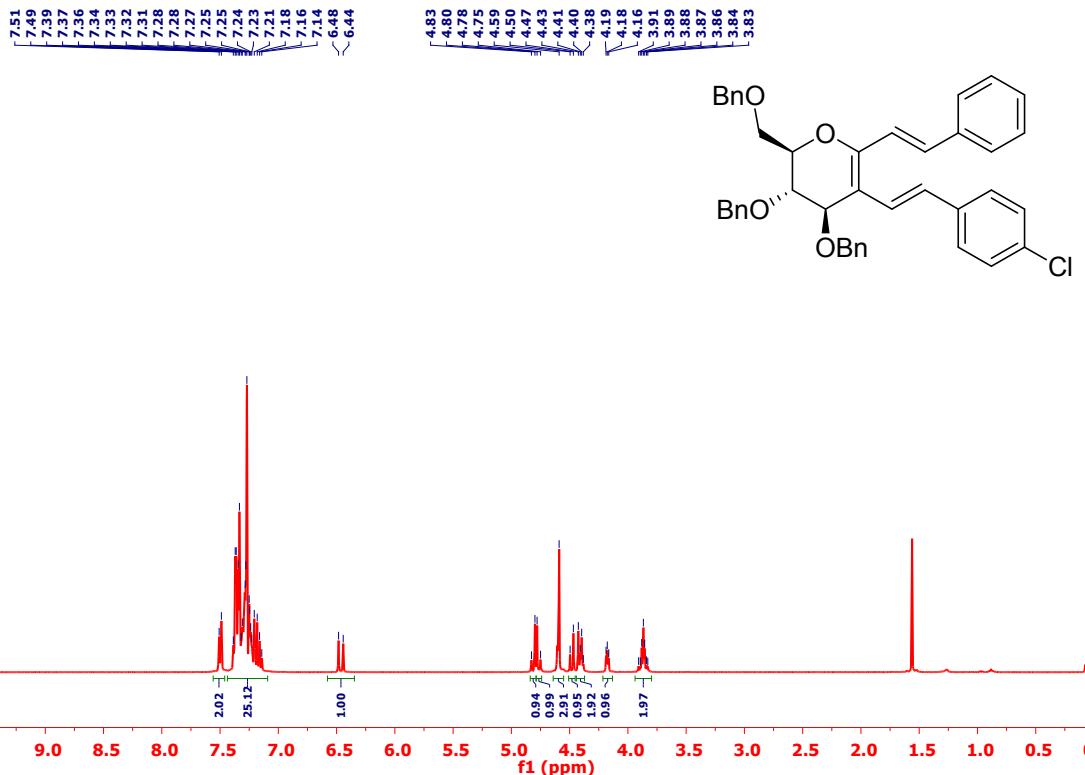


Figure S8. ¹H NMR spectrum of compound 4c (400 MHz, CDCl₃)

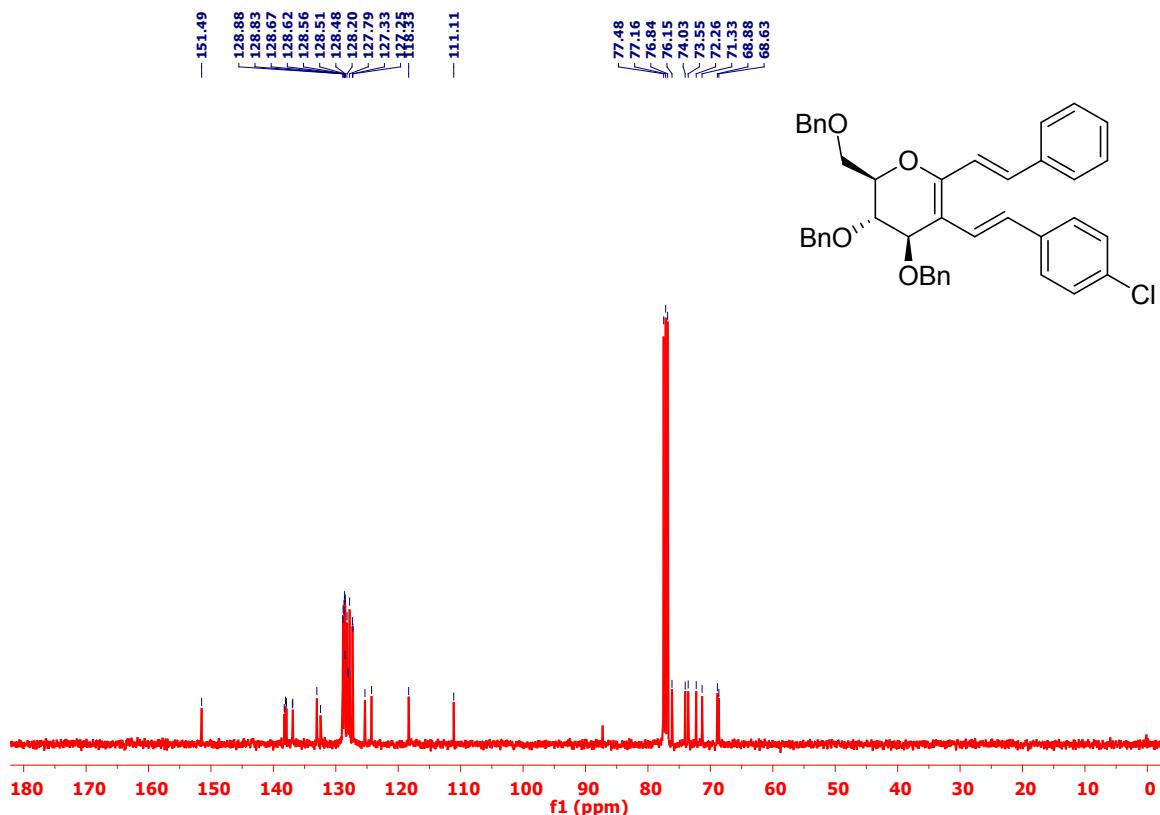


Figure S9. ¹³C NMR spectrum of compound 4c (100.6 MHz, CDCl₃)

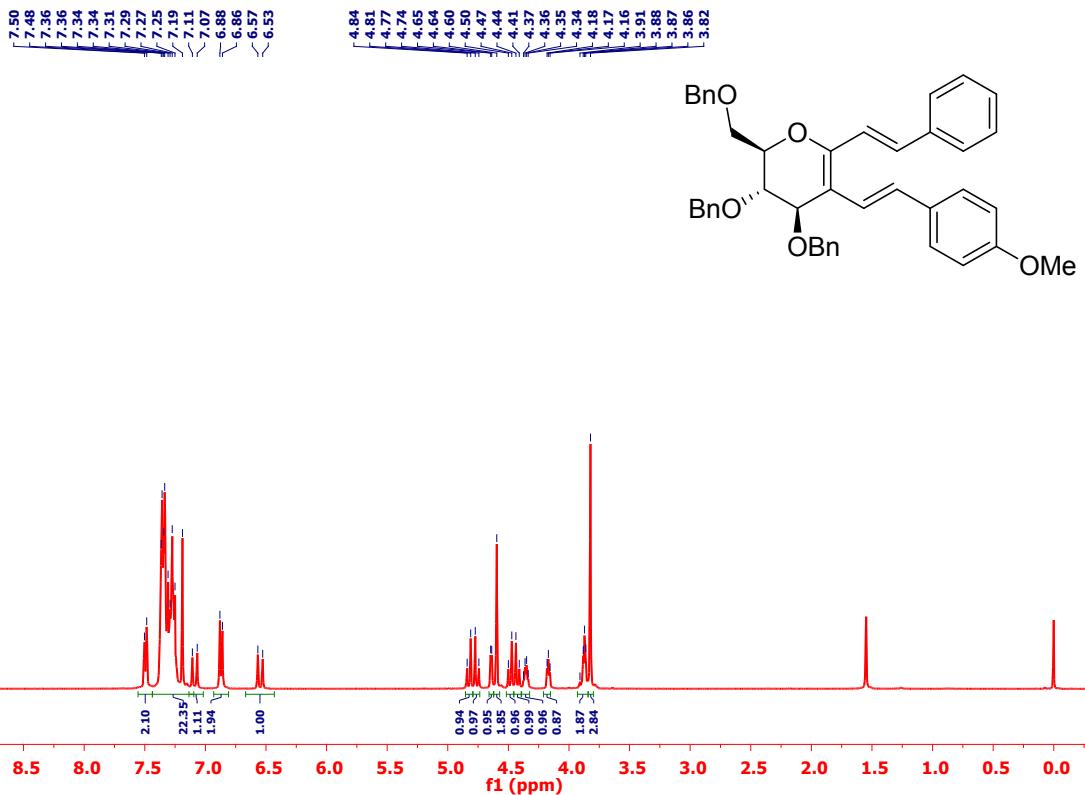


Figure S10. ¹H NMR spectrum of compound **4d** (400 MHz, CDCl₃)

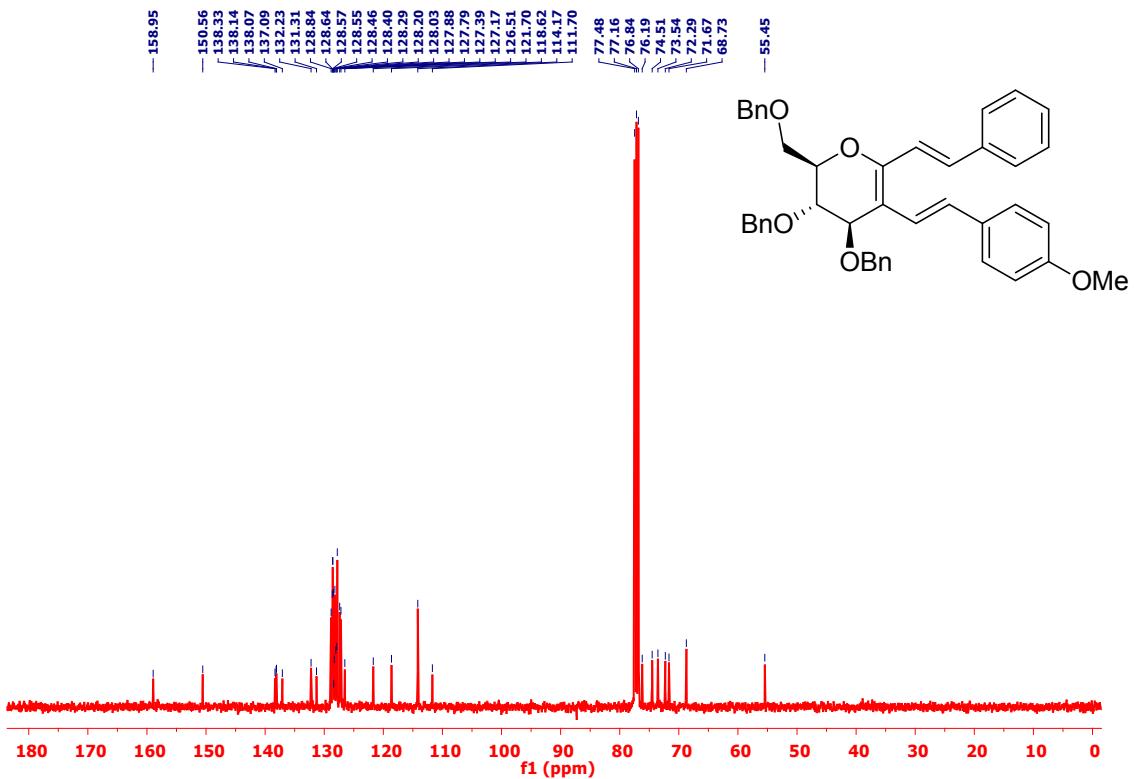


Figure S11. ¹³C NMR spectrum of compound **4d** (100.6 MHz, CDCl₃)

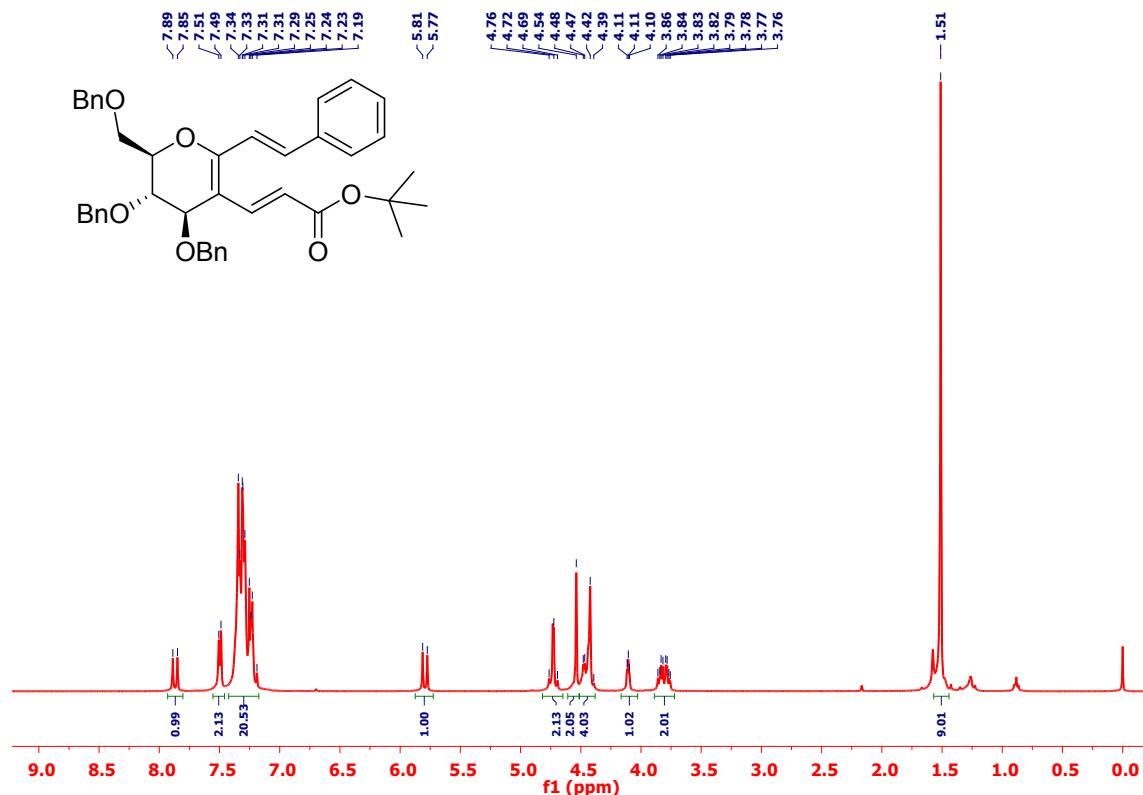


Figure S12. ¹H NMR spectrum of compound 4e (400 MHz, CDCl₃)

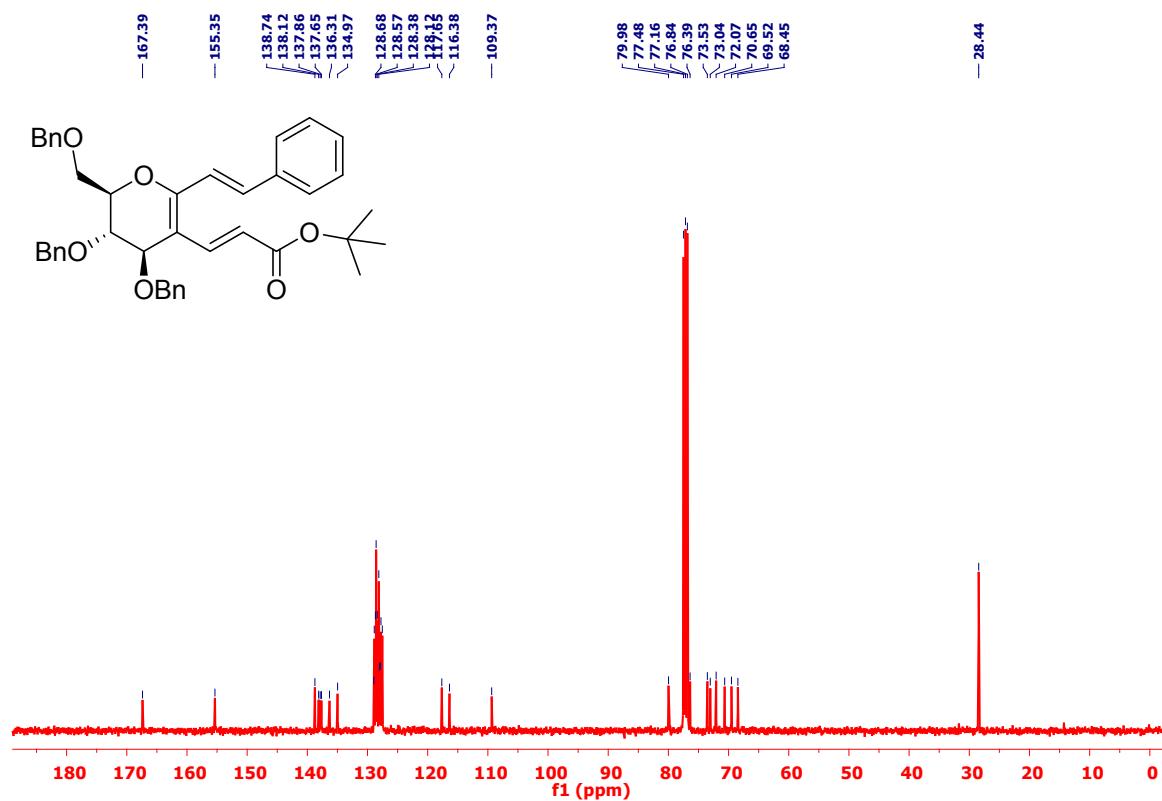


Figure S13. ¹³C NMR spectrum of compound 4e (100.6 MHz, CDCl₃)



Figure S14. ^1H NMR spectrum of compound **4f** (400 MHz, CDCl_3)

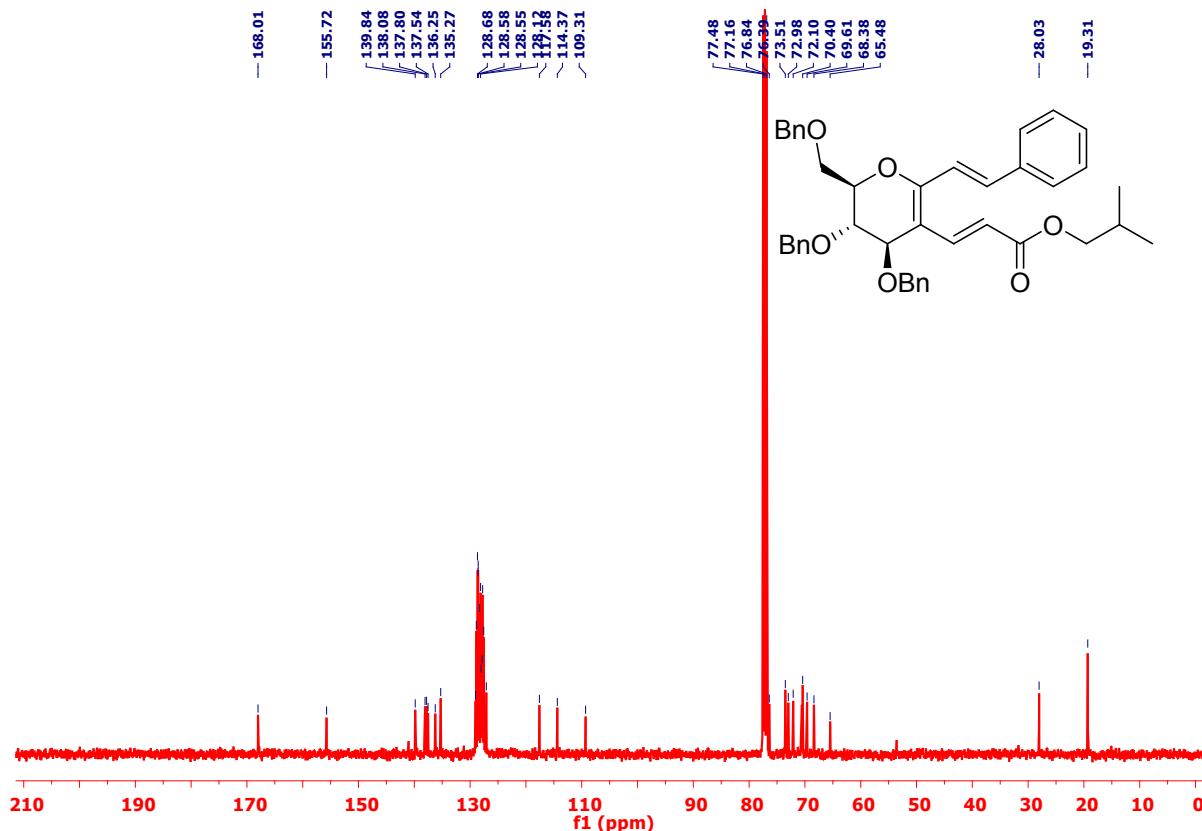


Figure S15. ^{13}C NMR spectrum of compound **4f** (100.6 MHz, CDCl_3)

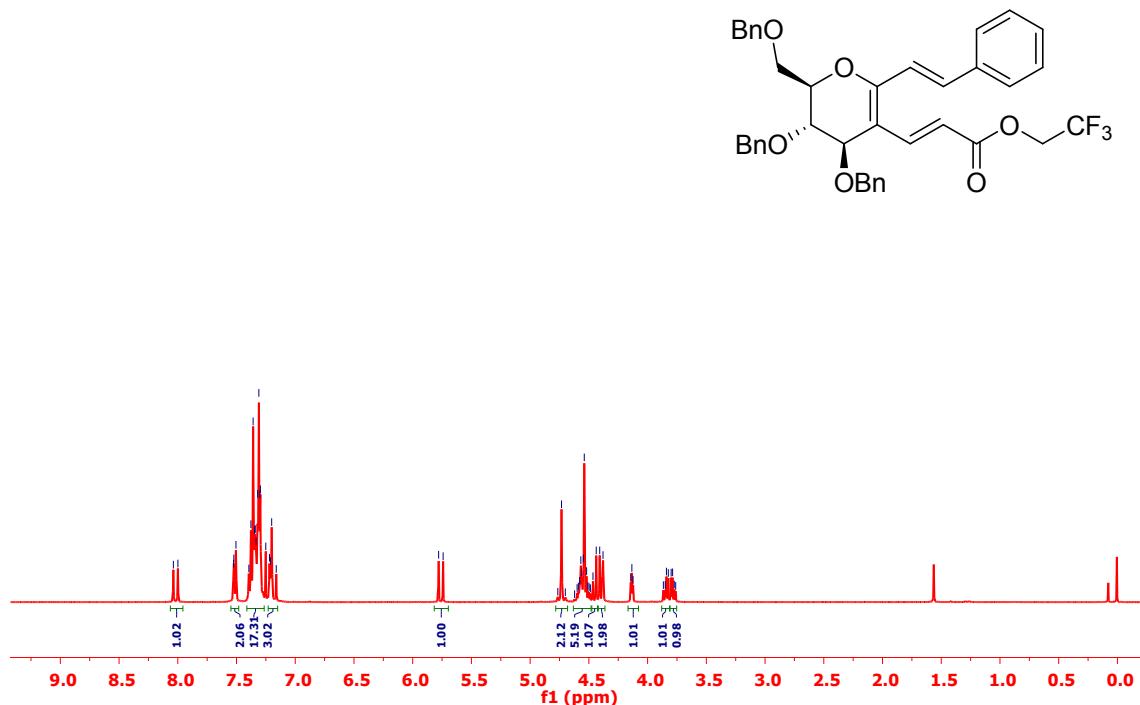


Figure S16. ¹H NMR spectrum of compound 4g (400 MHz, CDCl₃)

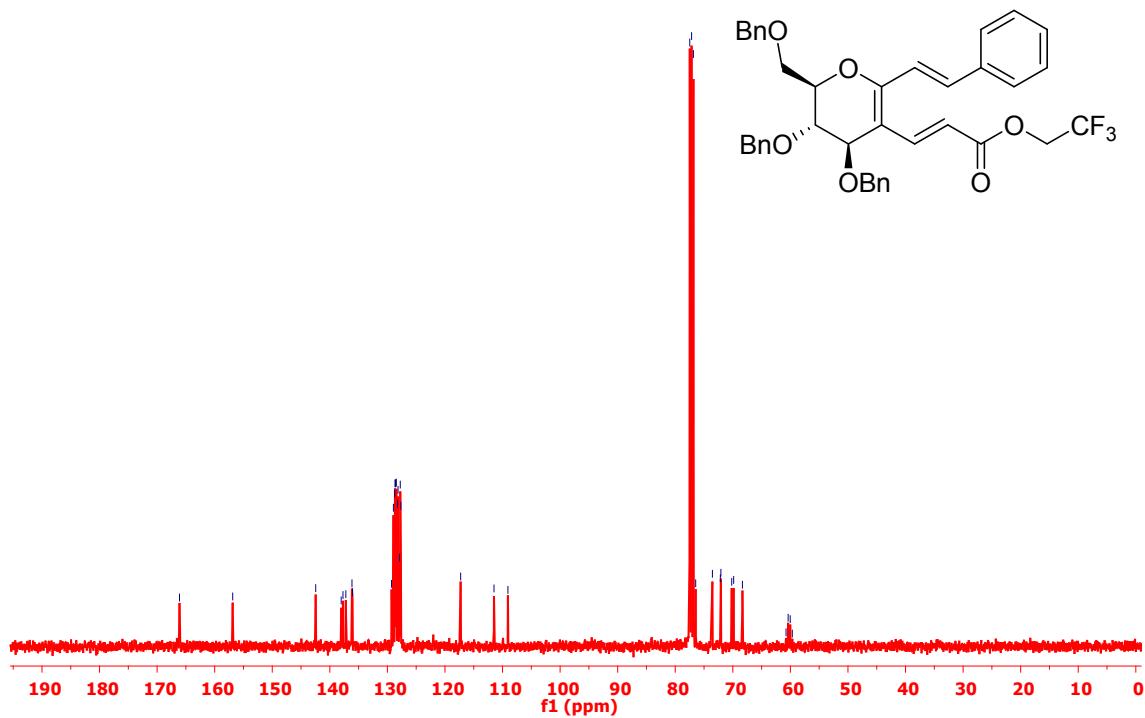


Figure S17. ¹³C NMR spectrum of compound 4g (100.6 MHz, CDCl₃)

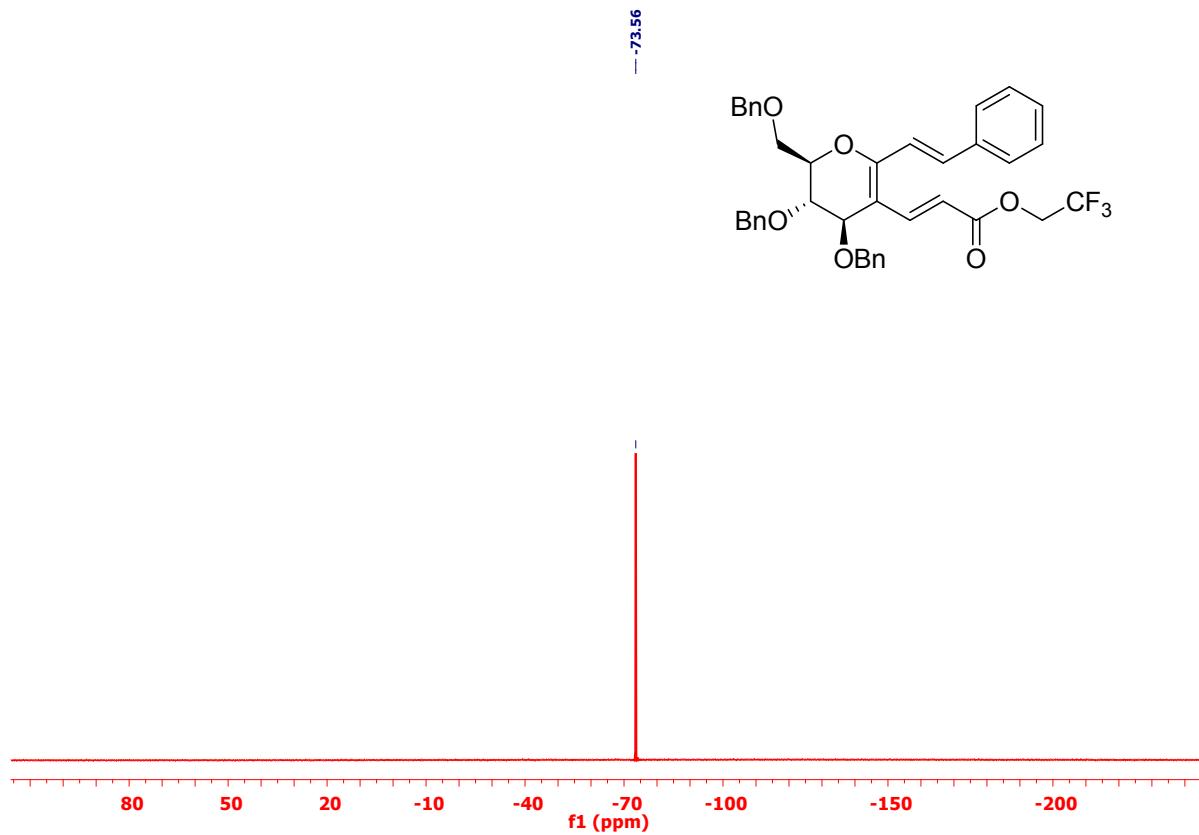


Figure S18. ¹⁹F NMR spectrum of compound **4g** (376 MHz, CDCl₃)

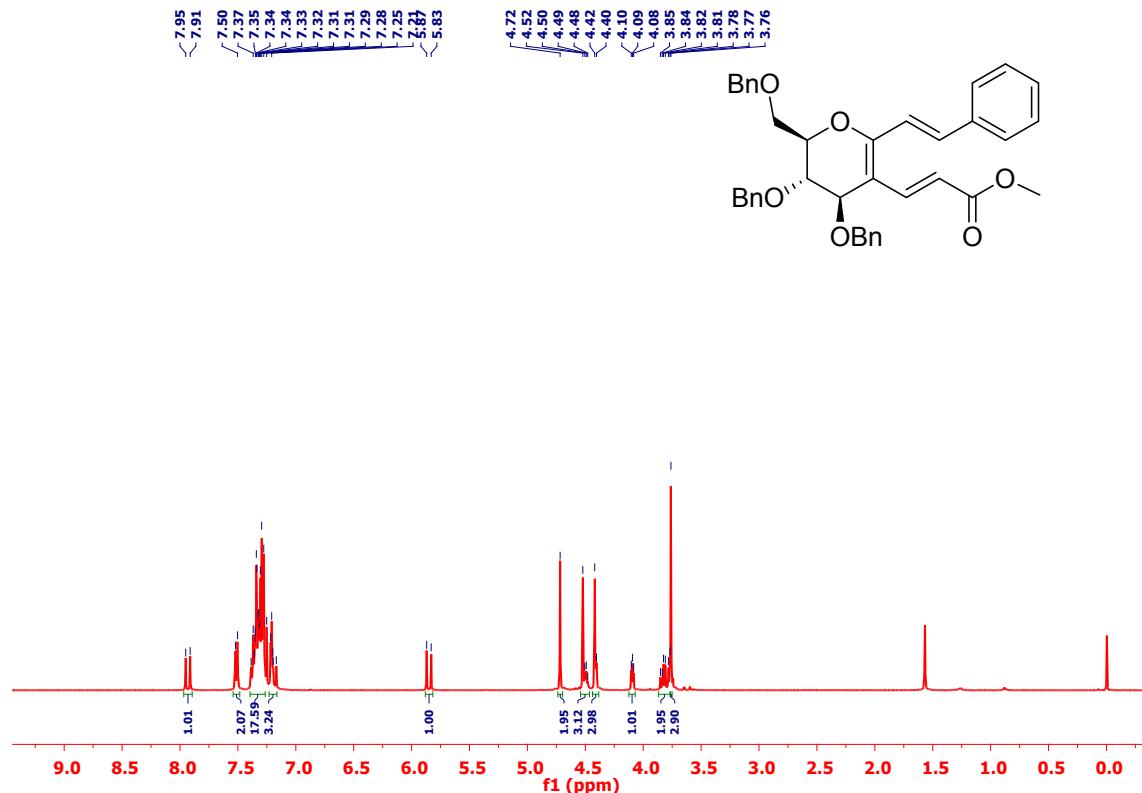


Figure S19. ¹H NMR spectrum of compound **4h** (400 MHz, CDCl_3)

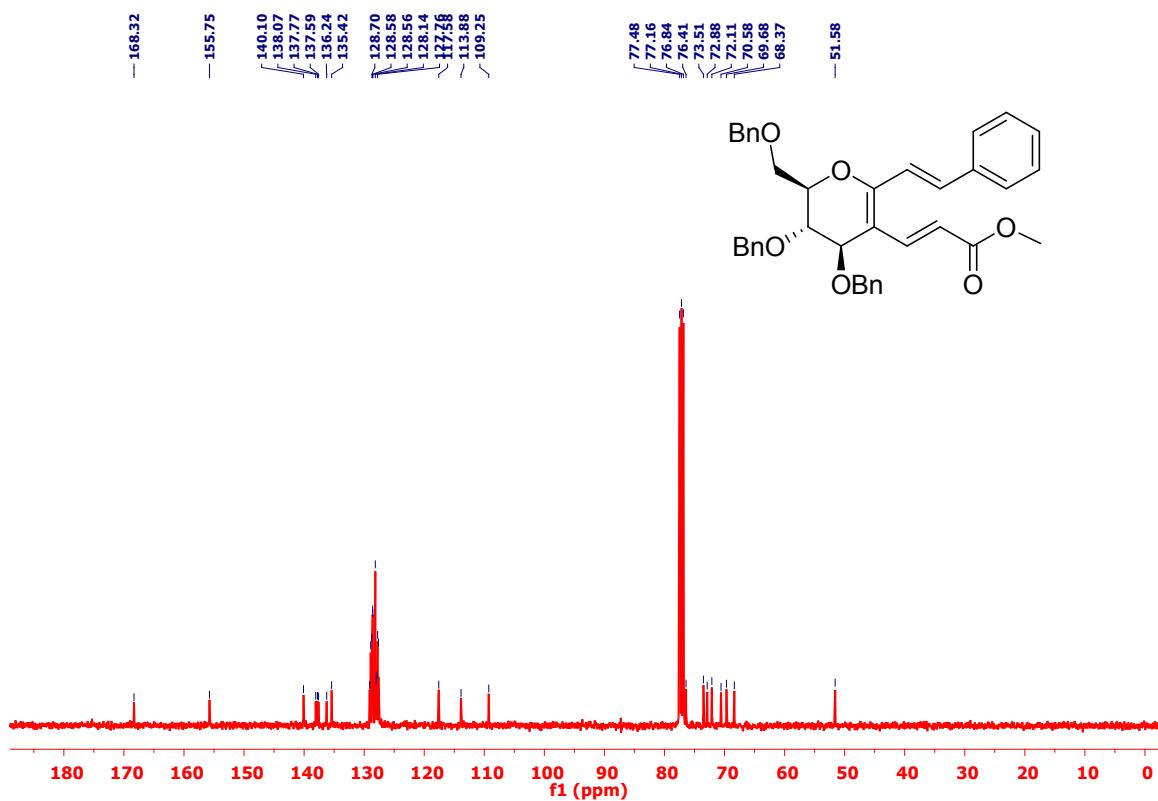


Figure S20. ¹³C NMR spectrum of compound **4h** (100.6 MHz, CDCl_3)

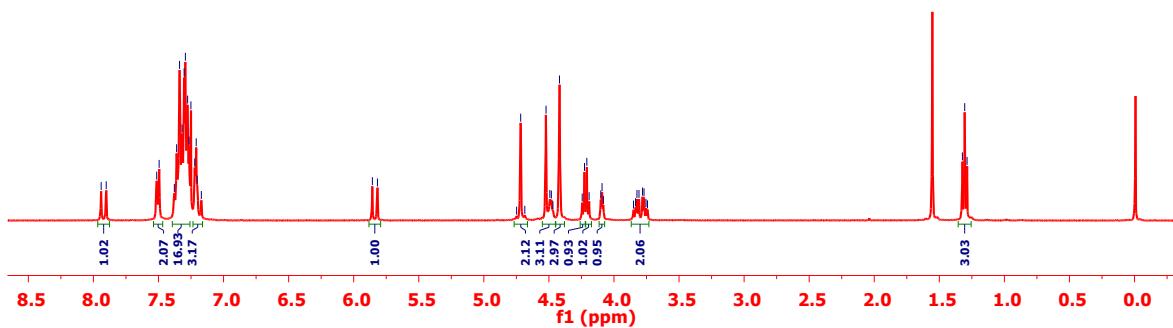
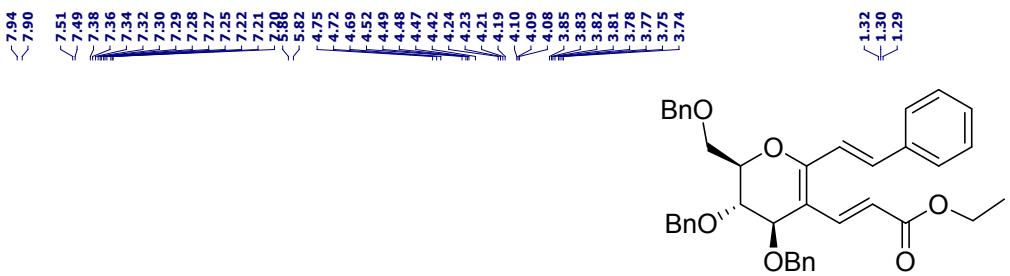


Figure S21. ¹H NMR spectrum of compound **4i** (400 MHz, CDCl₃)

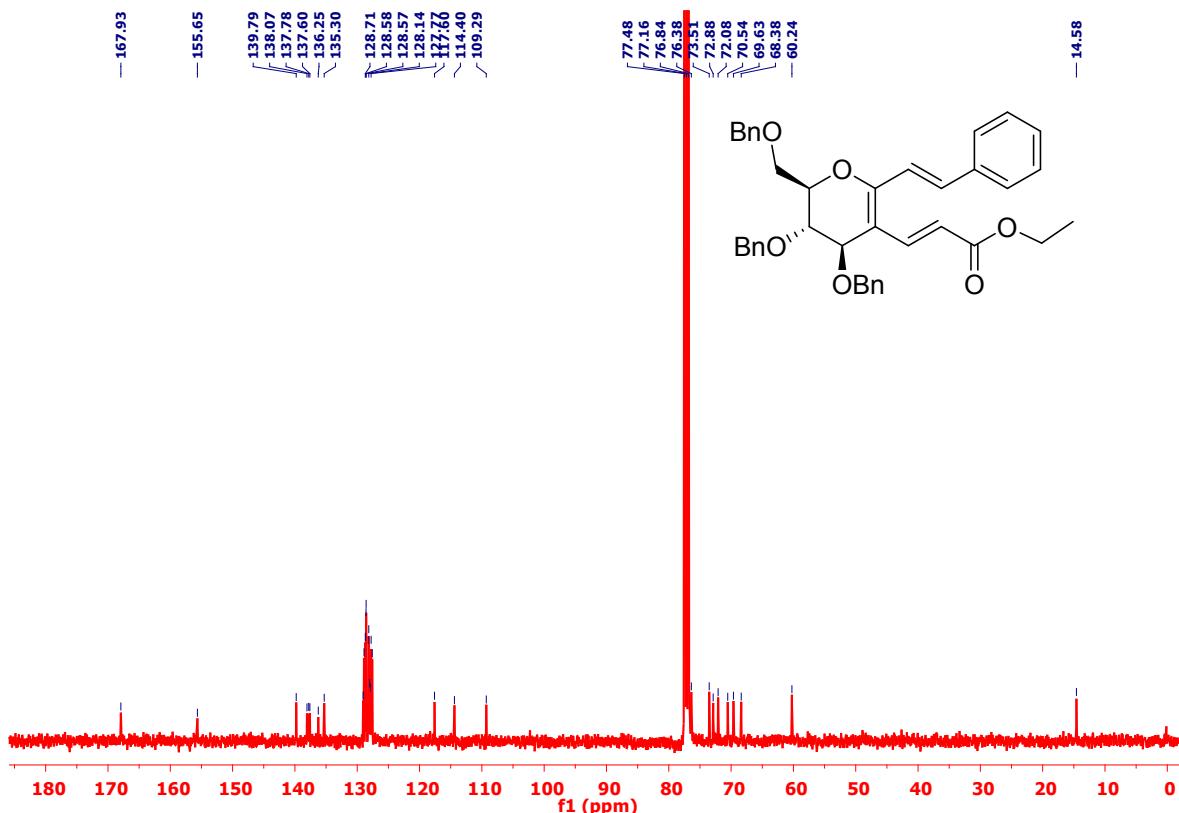


Figure S22. ¹³C NMR spectrum of compound **4i** (100.6 MHz, CDCl₃)

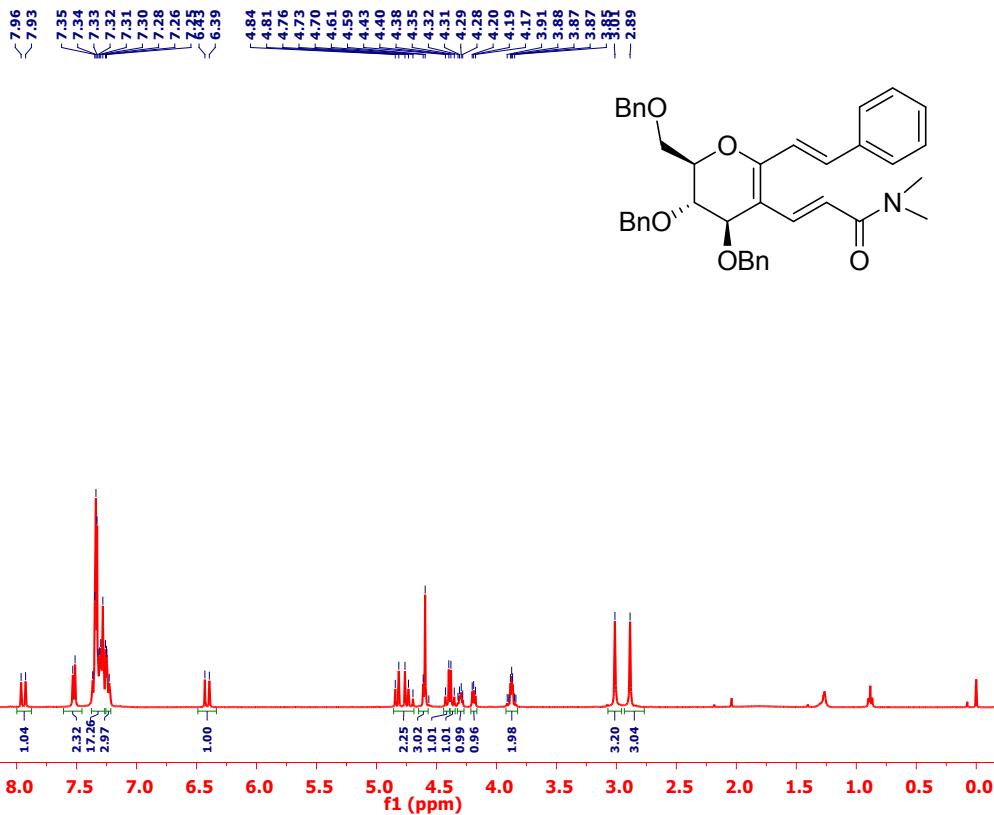


Figure S23. ¹H NMR spectrum of compound **4j** (400 MHz, CDCl₃)

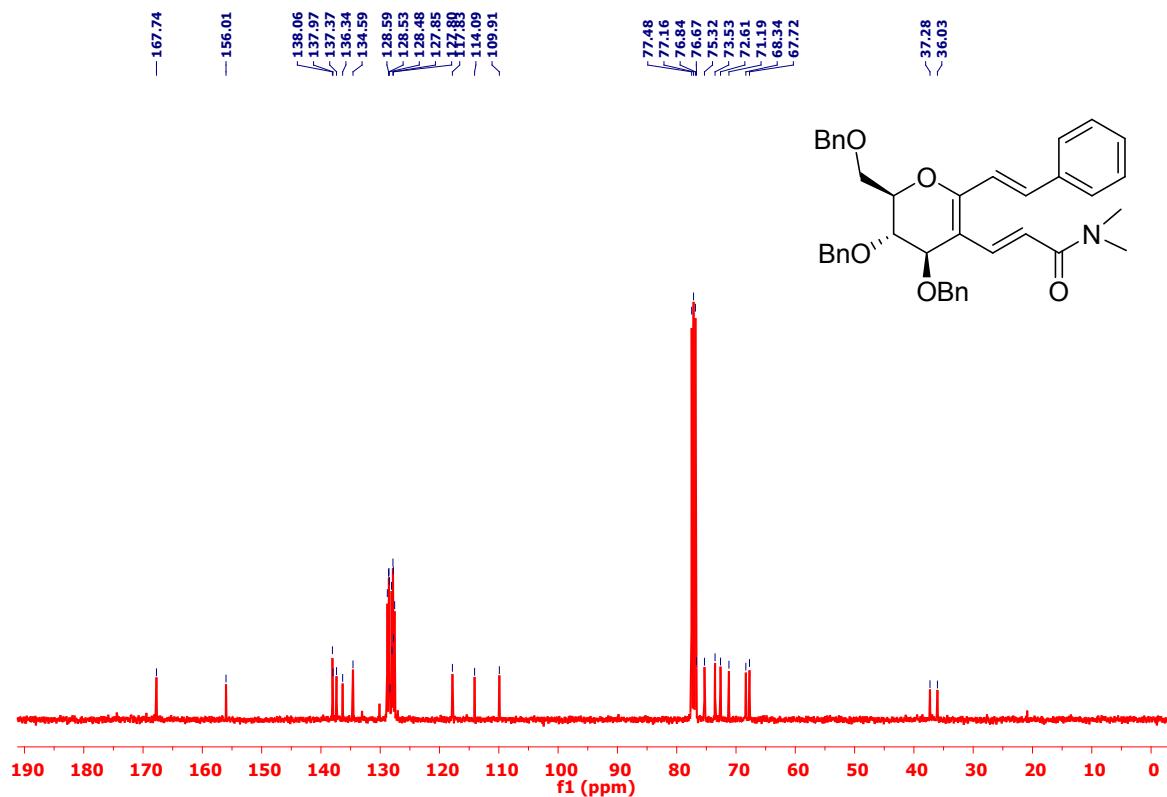


Figure S24. ¹³C NMR spectrum of compound **4j** (100.6 MHz, CDCl₃)

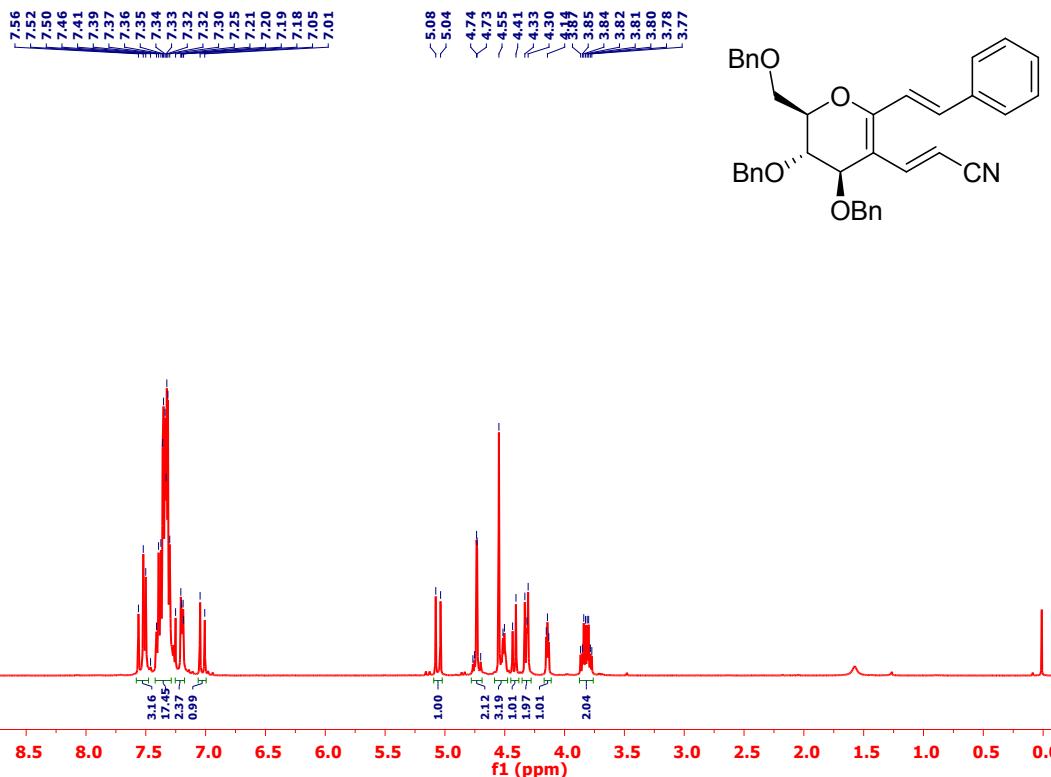


Figure S25. ¹H NMR spectrum of compound **4k** (400 MHz, CDCl₃)

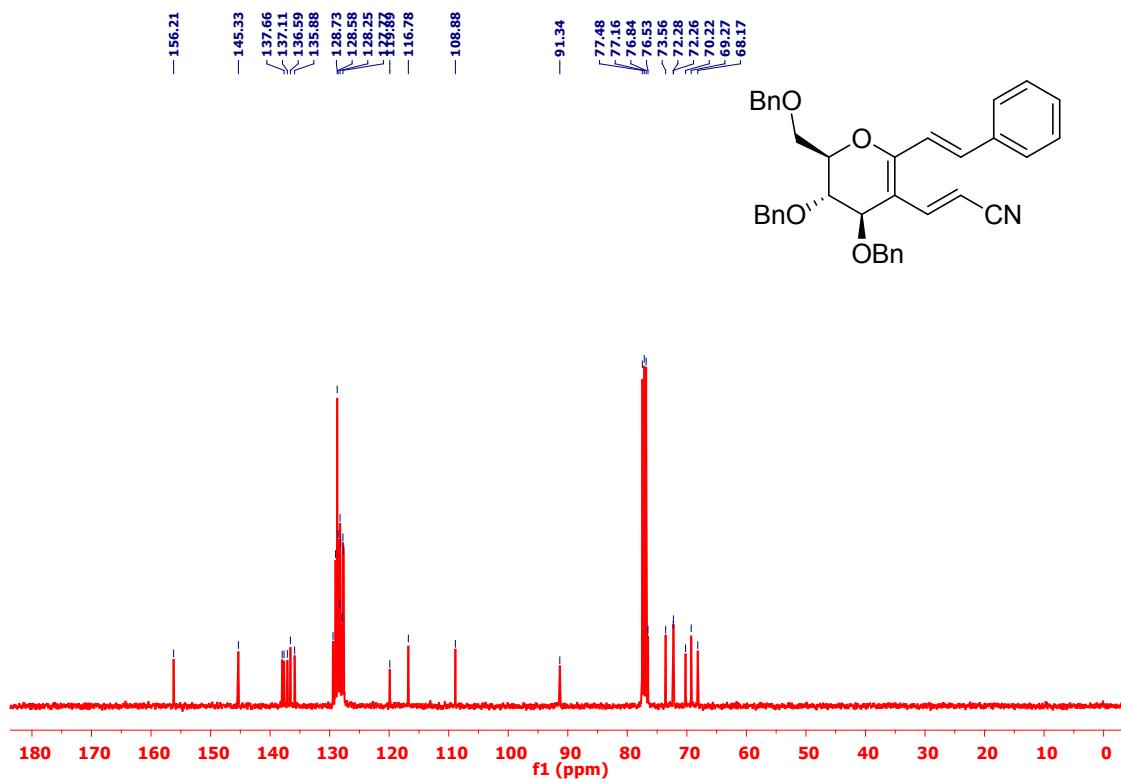


Figure S26. ¹³C NMR spectrum of compound **4k** (100.6 MHz, CDCl₃)

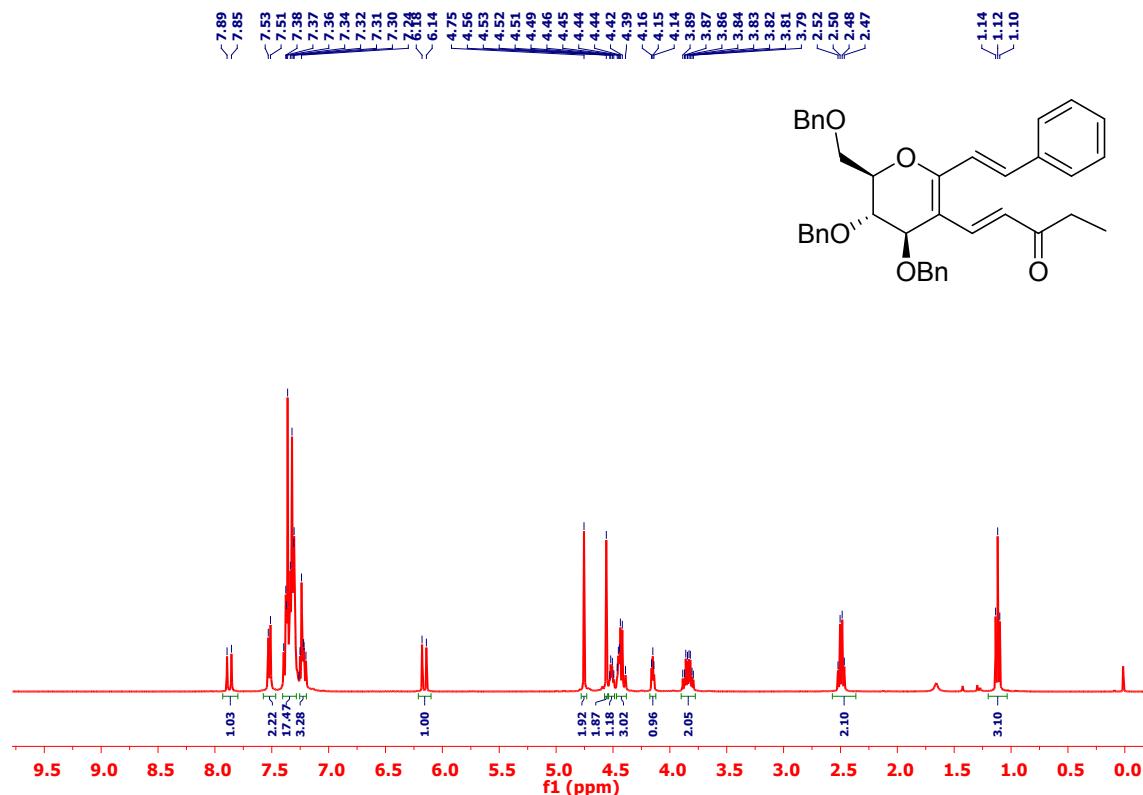


Figure S27. ¹H NMR spectrum of compound 4l (400 MHz, CDCl₃)

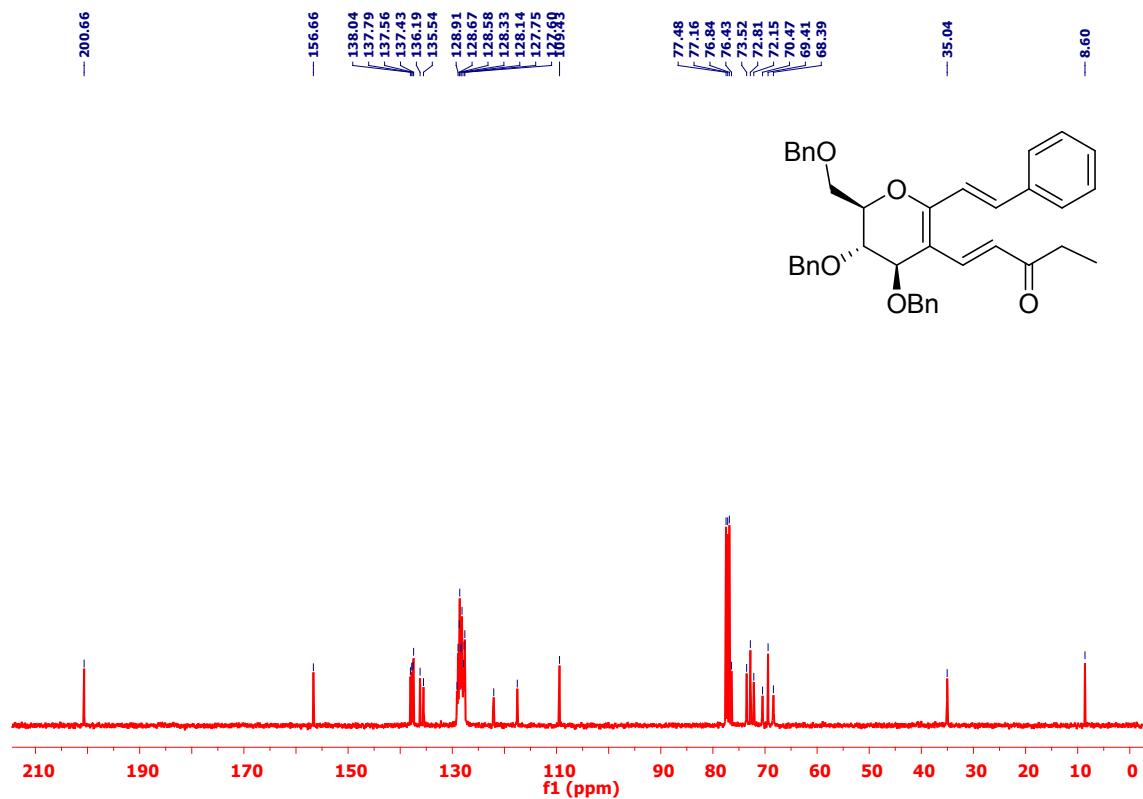


Figure S28. ¹³C NMR spectrum of compound 4l (100.6 MHz, CDCl₃)

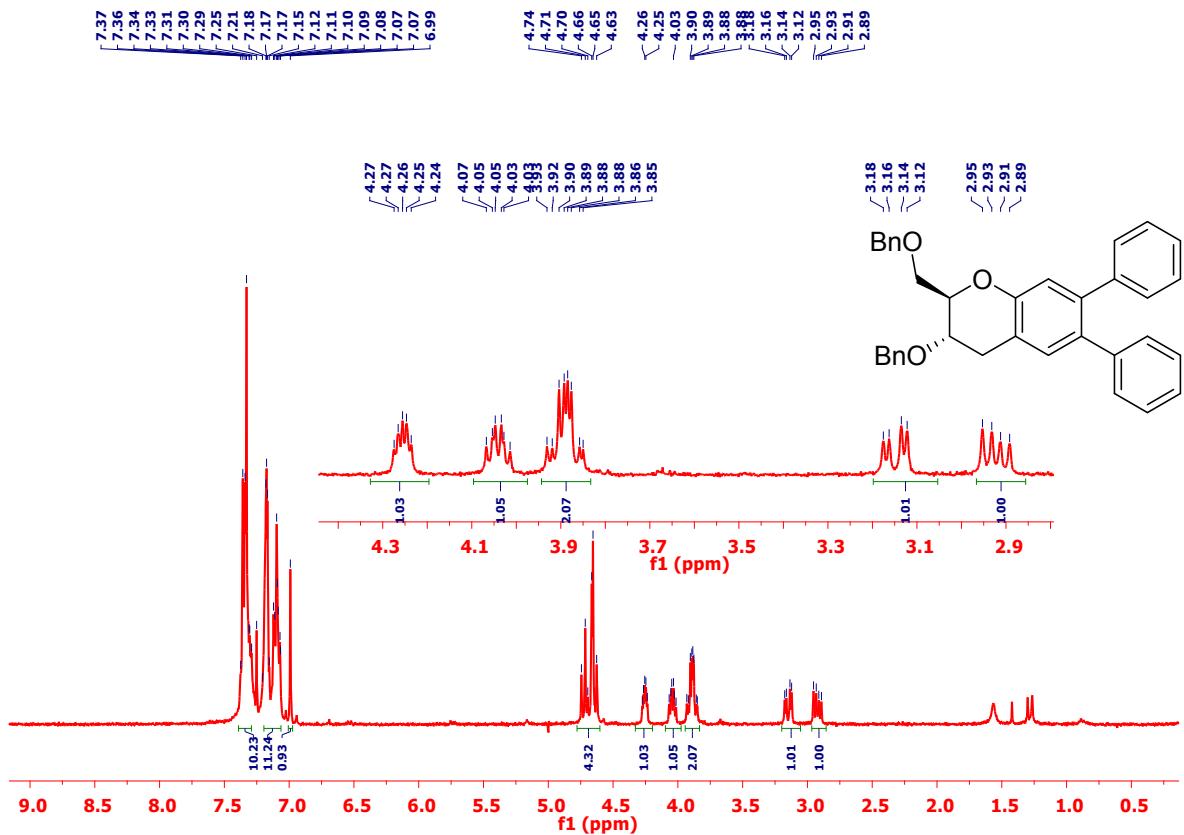


Figure S29. ¹H NMR spectrum of compound 5a (400 MHz, CDCl₃)

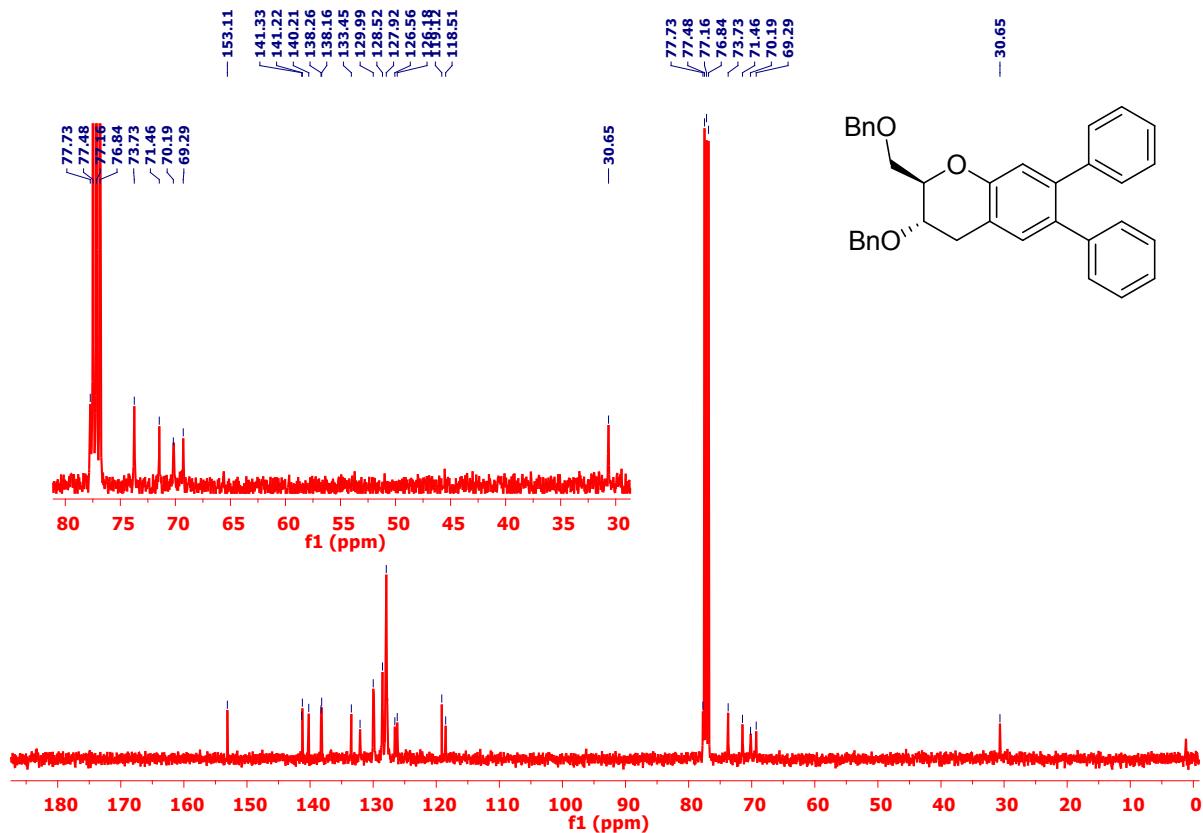


Figure S30. ¹³C NMR spectrum of compound 5a (100.6 MHz, CDCl₃)

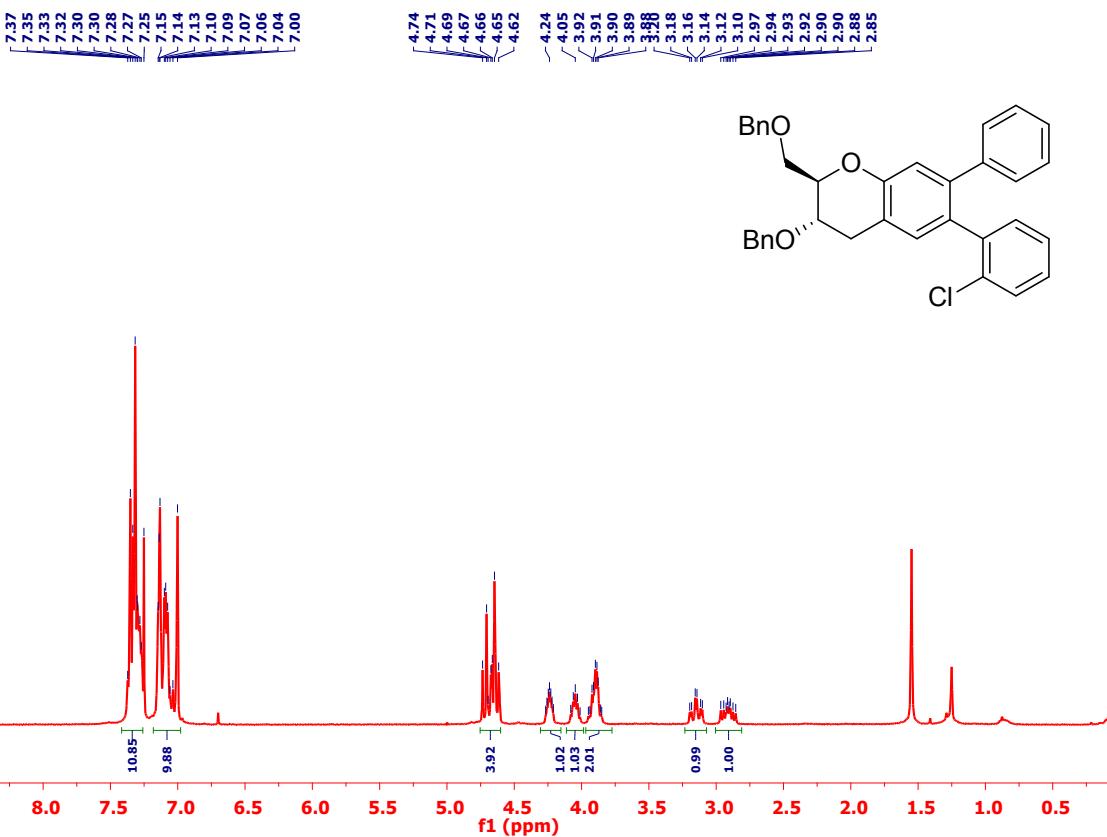


Figure S31. ¹H NMR spectrum of compound **5b** (400 MHz, CDCl₃)

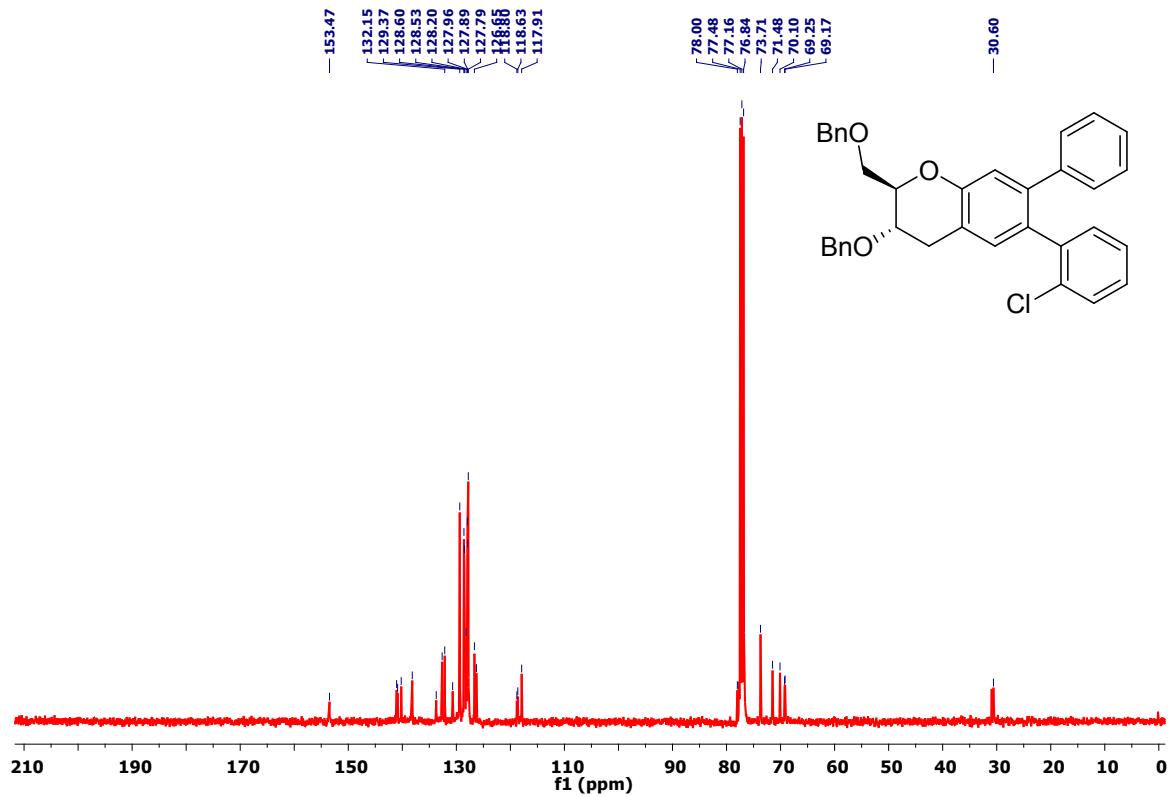


Figure S32. ¹³C NMR spectrum of compound **5b** (100.6 MHz, CDCl₃)

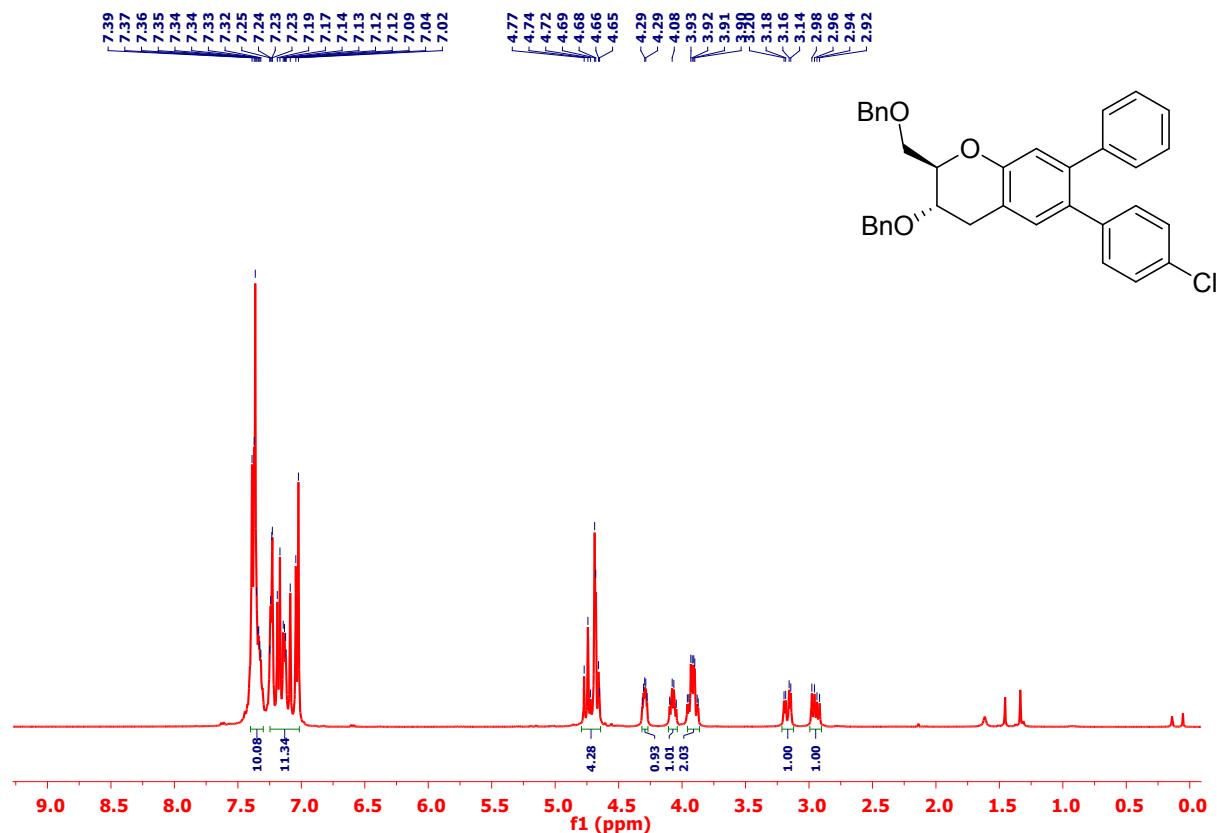


Figure S33. ¹H NMR spectrum of compound **5c** (400 MHz, CDCl₃)

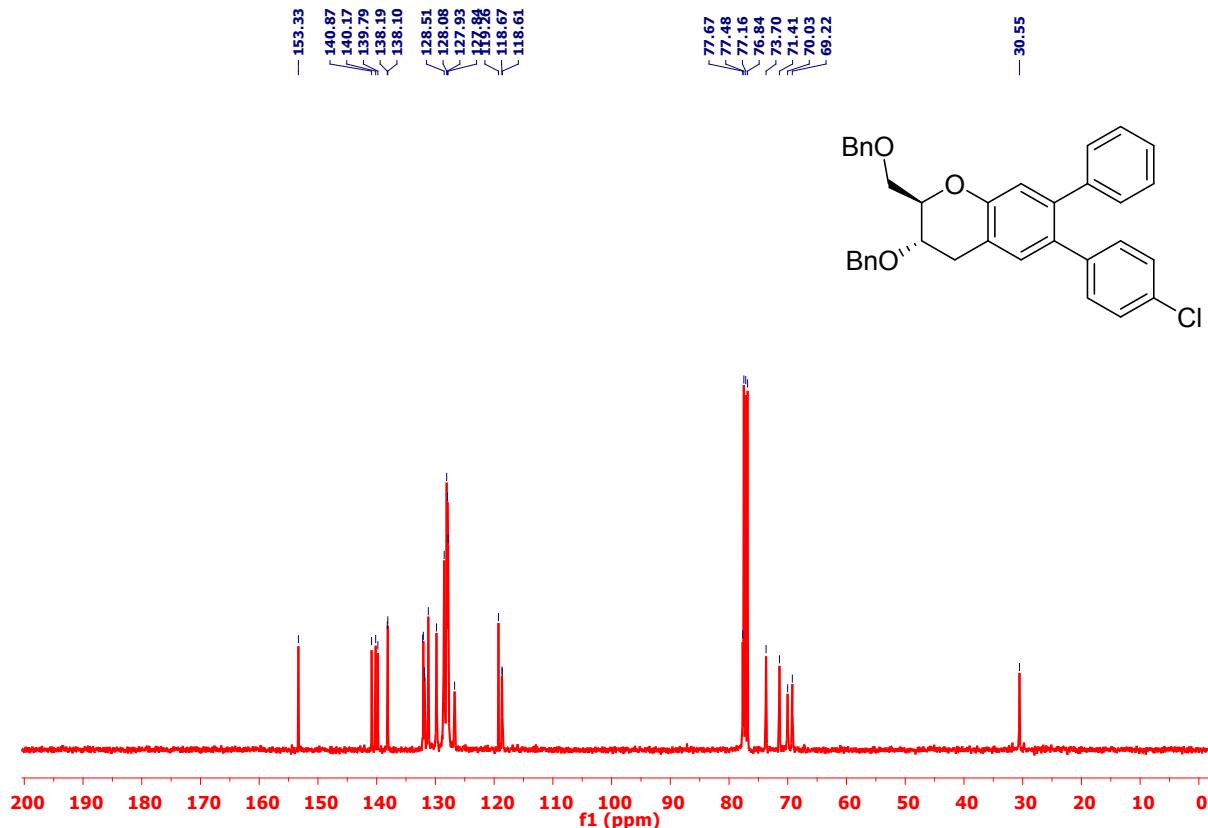


Figure S34. ¹³C NMR spectrum of compound **5c** (100.6 MHz, CDCl₃)

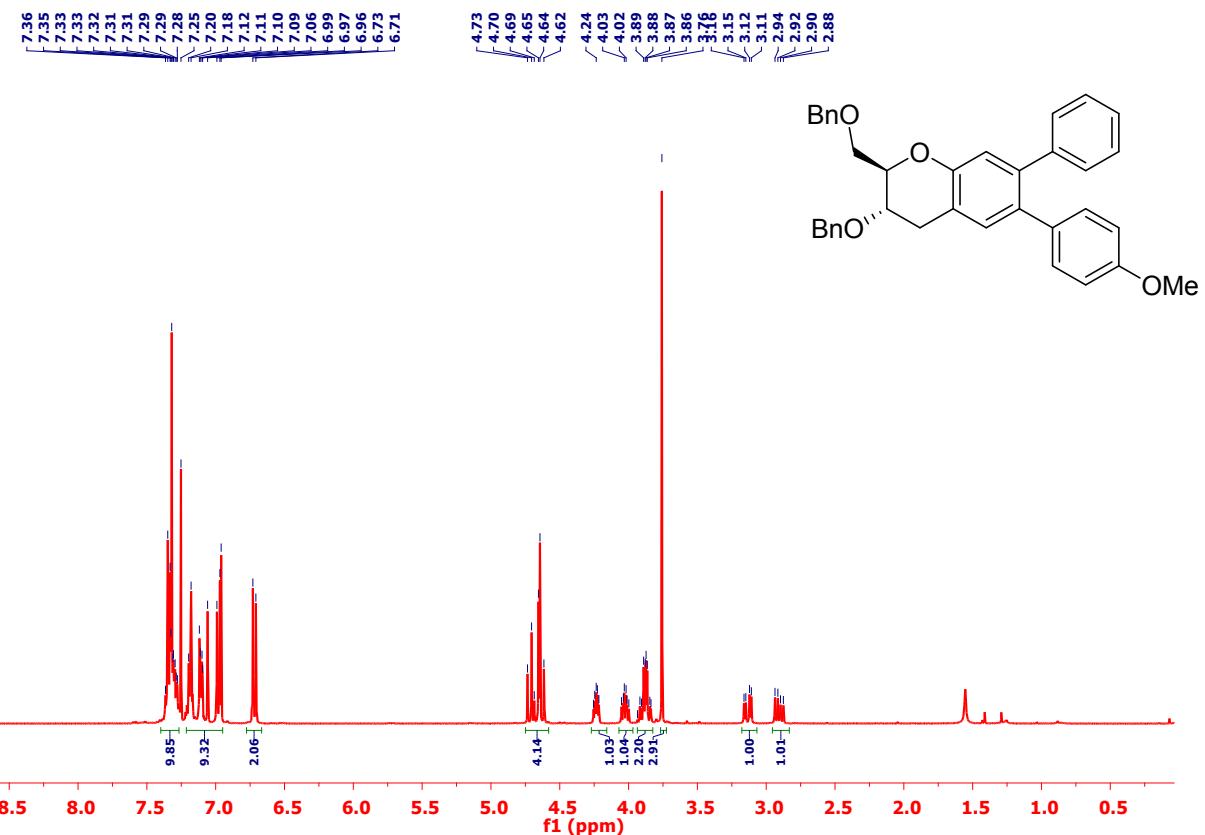


Figure S35. ¹H NMR spectrum of compound **5d** (400 MHz, CDCl₃)

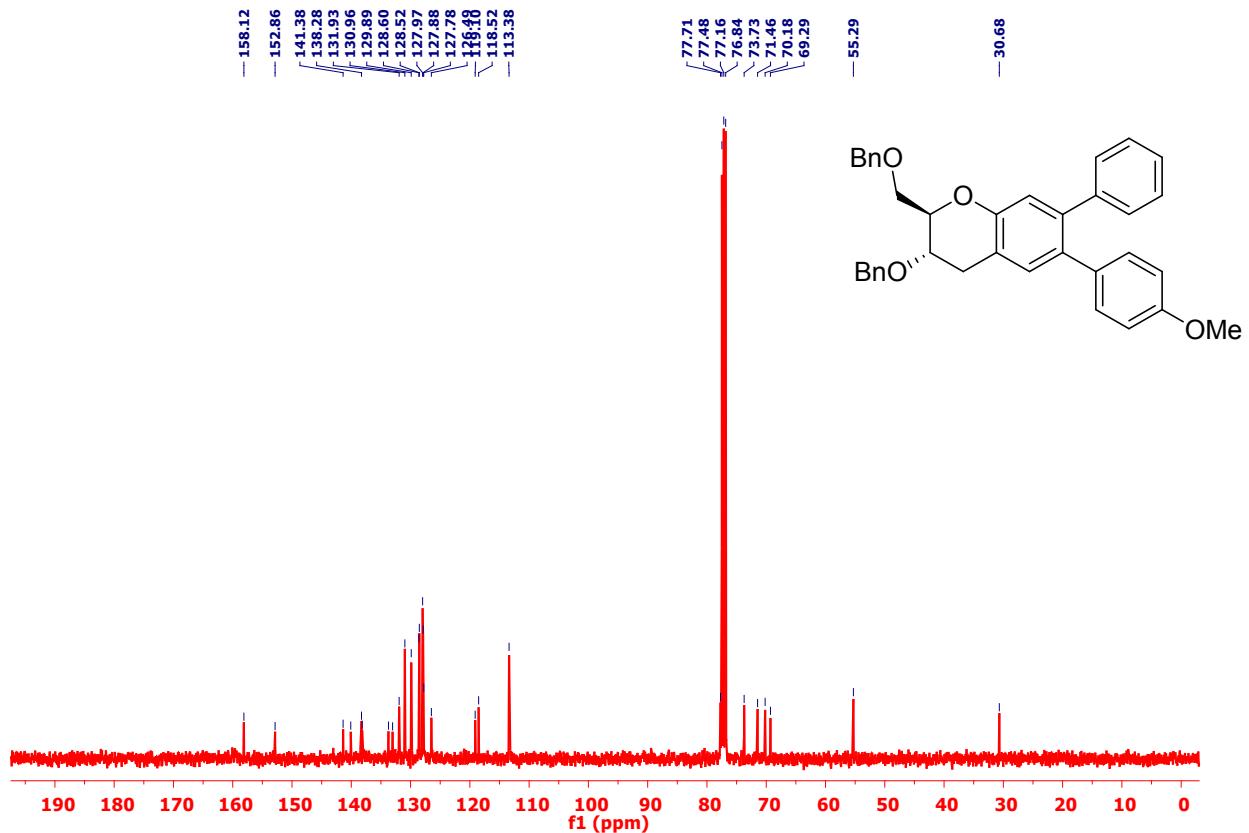


Figure S36. ¹³C NMR spectrum of compound **5d** (100.6 MHz, CDCl₃)

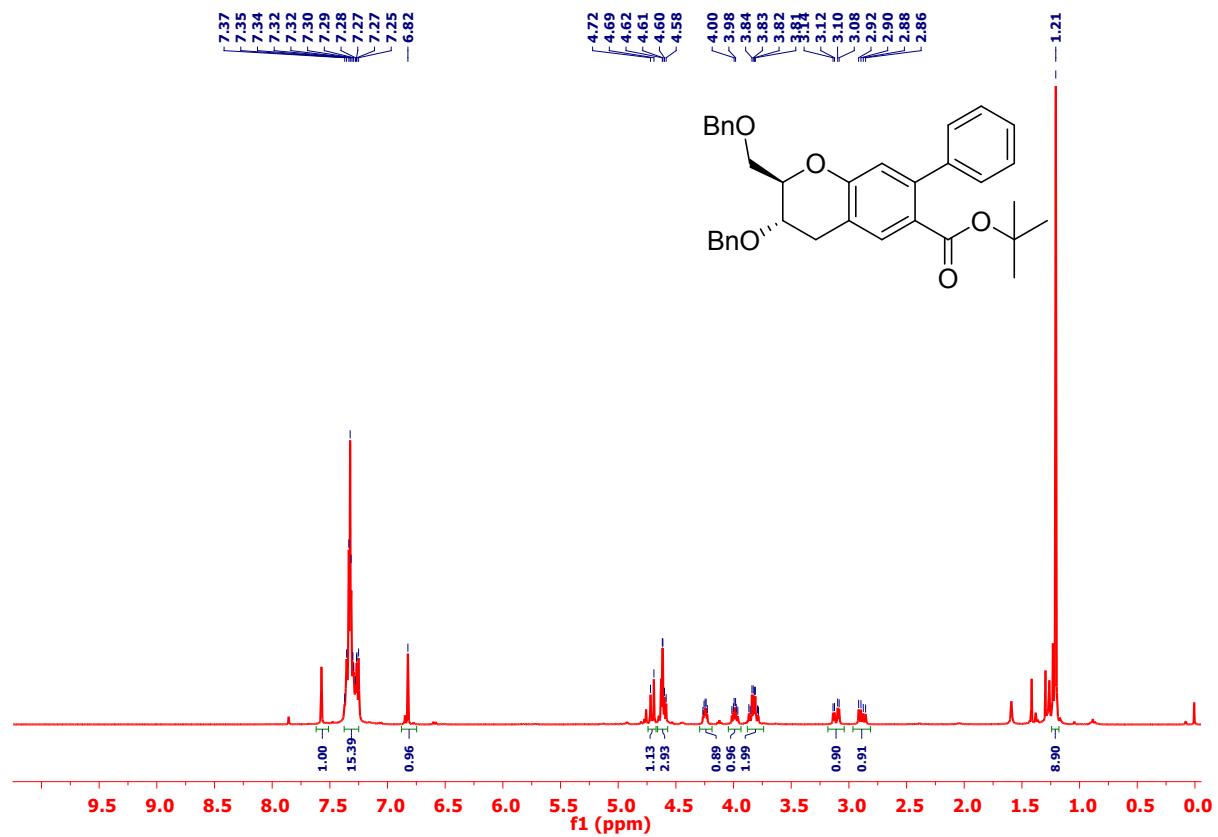


Figure S37. ¹H NMR spectrum of compound **5e** (400 MHz, CDCl₃)

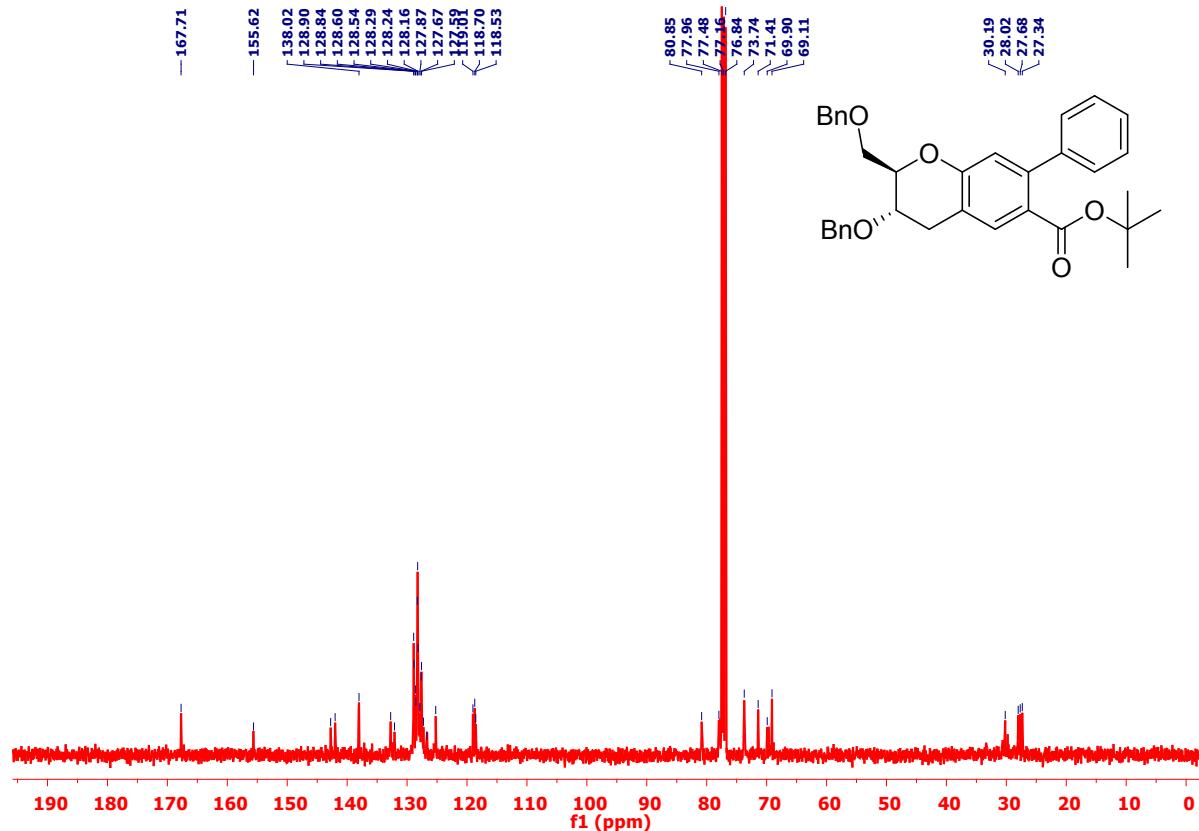


Figure S38. ¹³C NMR spectrum of compound **5e** (100.6 MHz, CDCl₃)

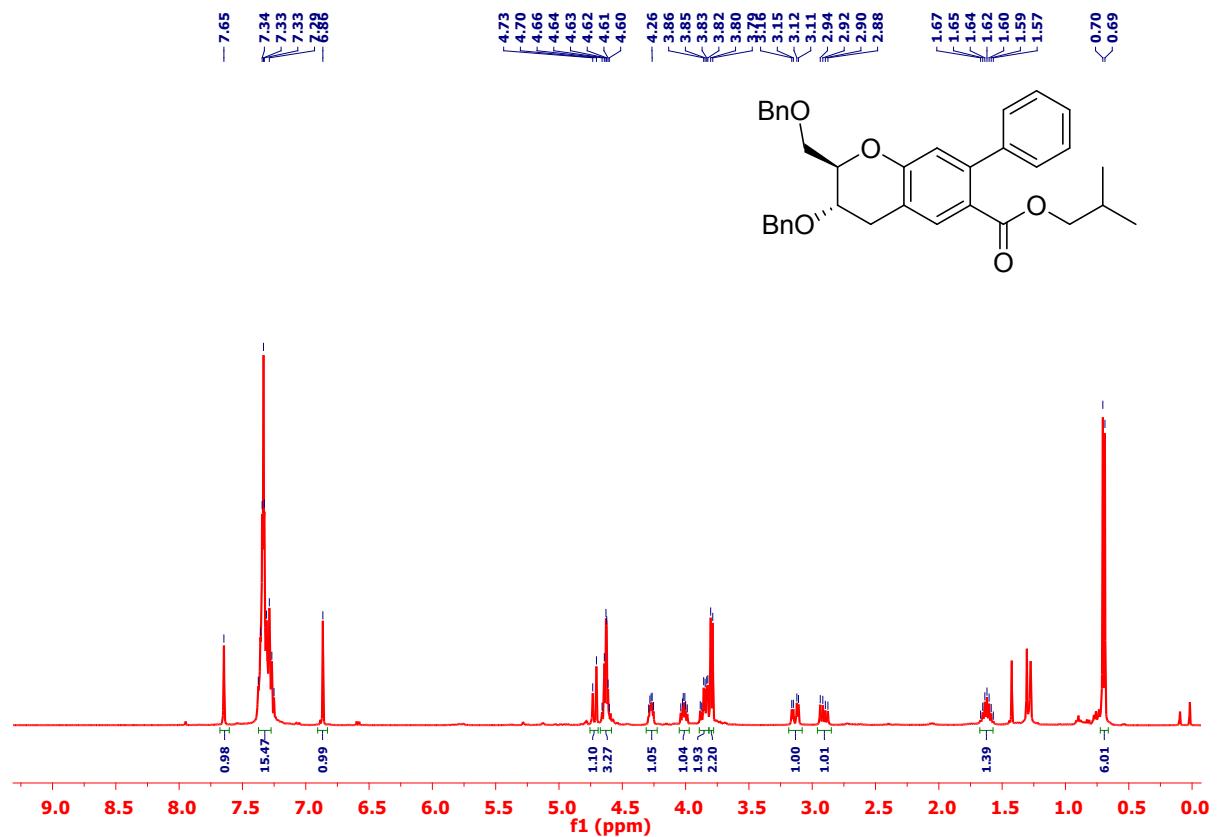


Figure S39. ¹H NMR spectrum of compound 5f (400 MHz, CDCl₃)

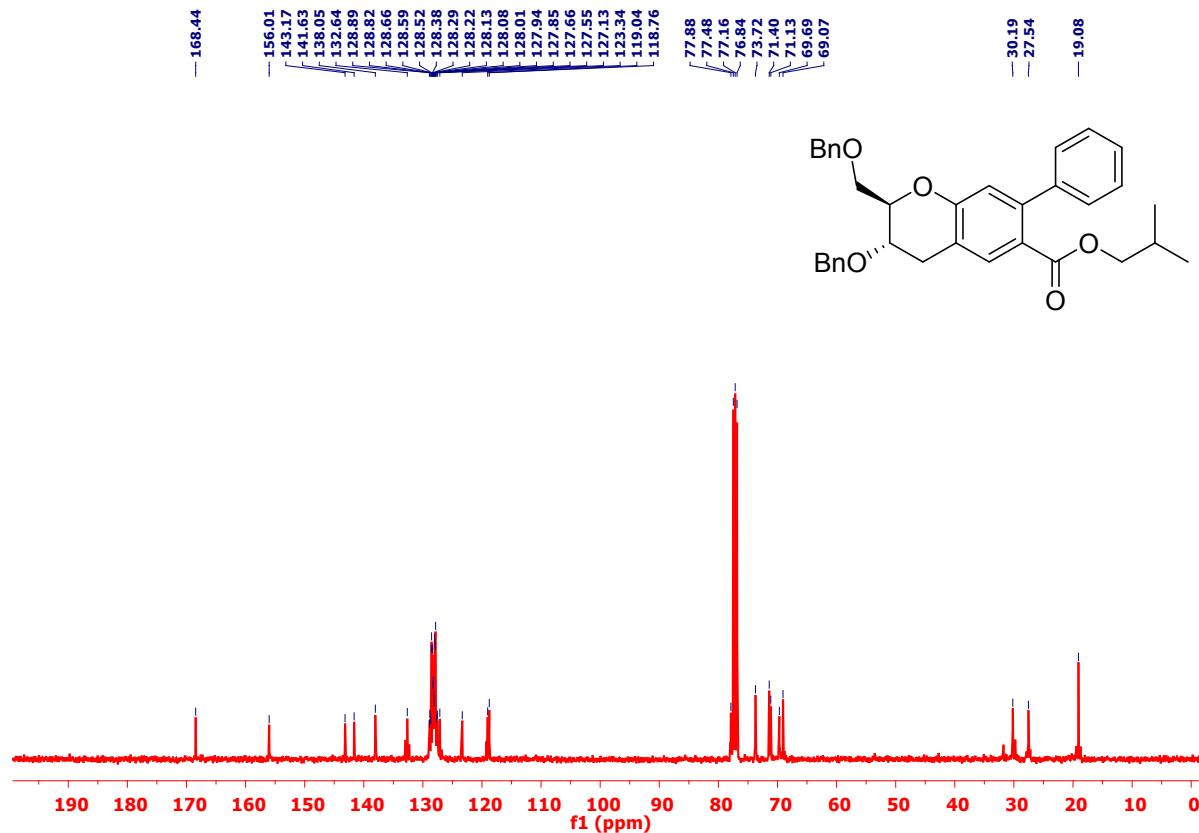


Figure S40. ¹³C NMR spectrum of compound 5f (100.6 MHz, CDCl₃)

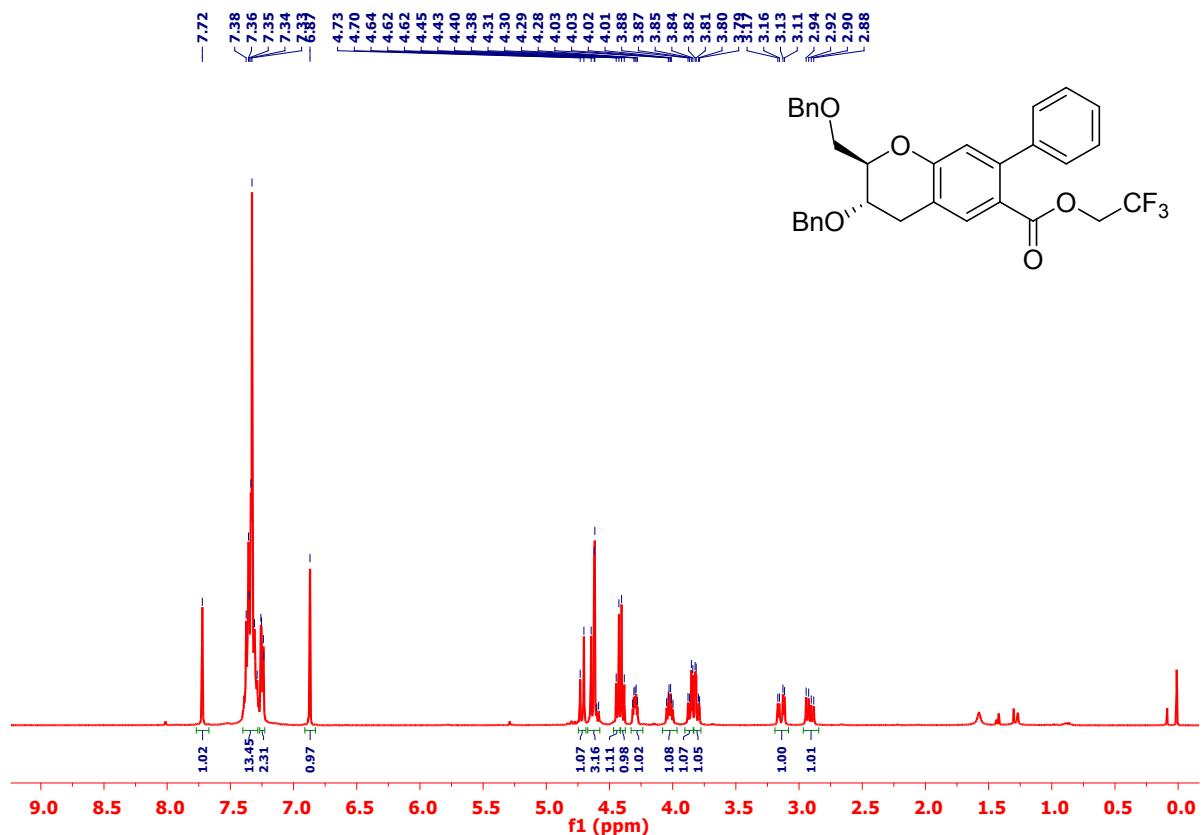


Figure S41. ¹H NMR spectrum of compound **5g** (400 MHz, CDCl₃)

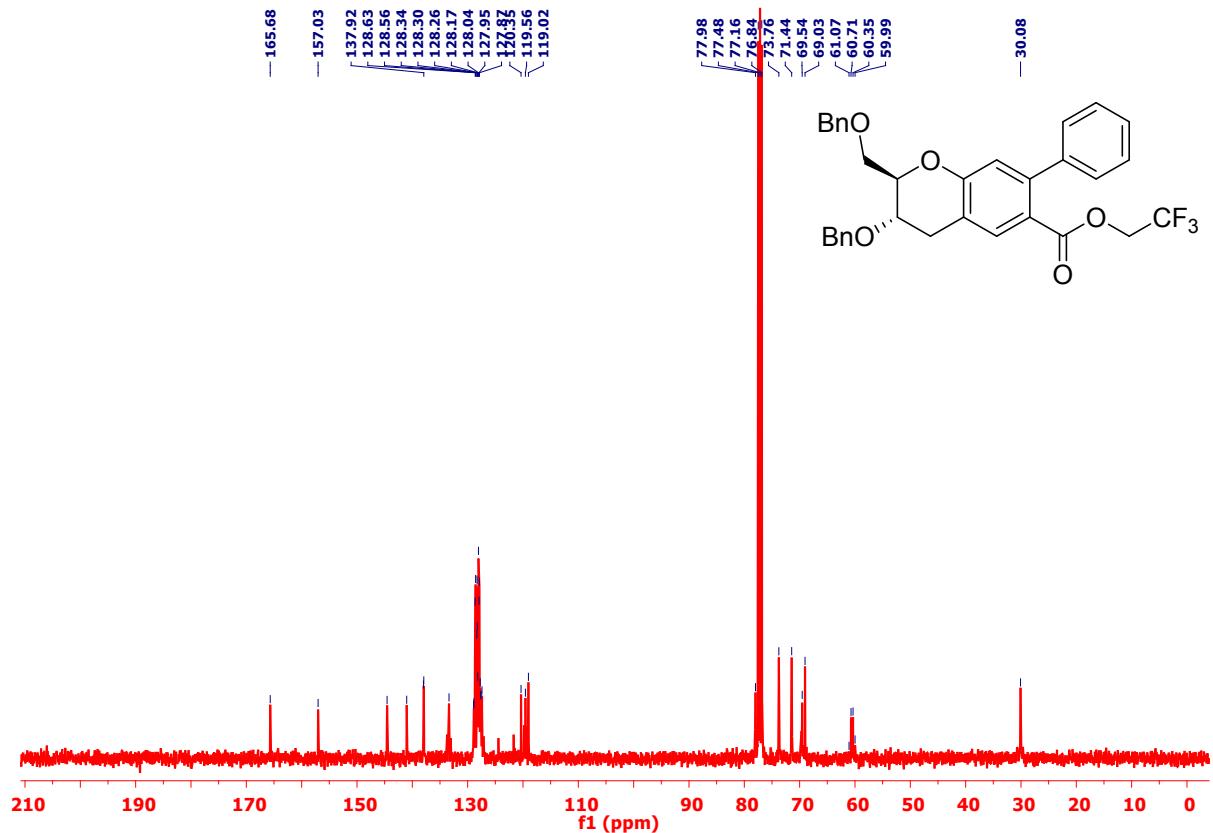


Figure S42. ¹³C NMR spectrum of compound **5g** (100.6 MHz, CDCl₃)

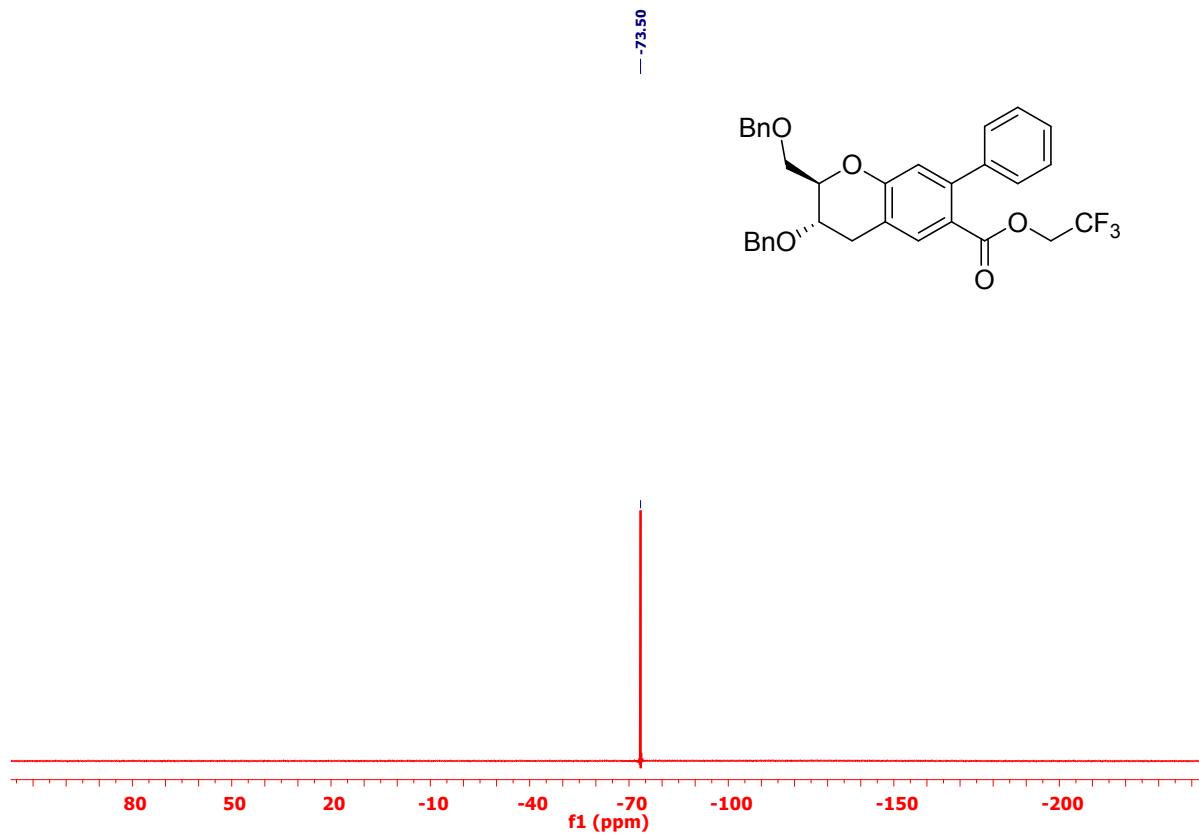


Figure S43. ¹⁹F NMR spectrum of compound **5g** (376 MHz, CDCl₃)

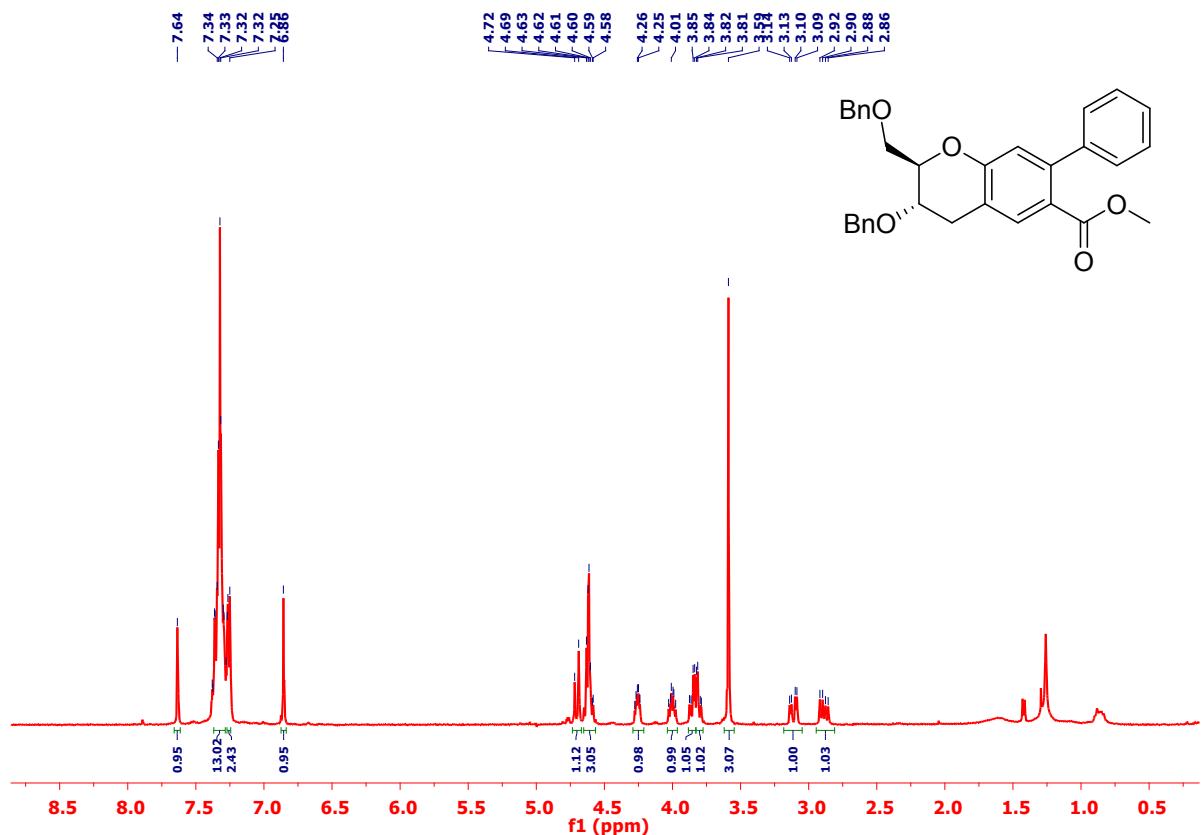


Figure S44. ¹H NMR spectrum of compound **5h** (400 MHz, CDCl₃)

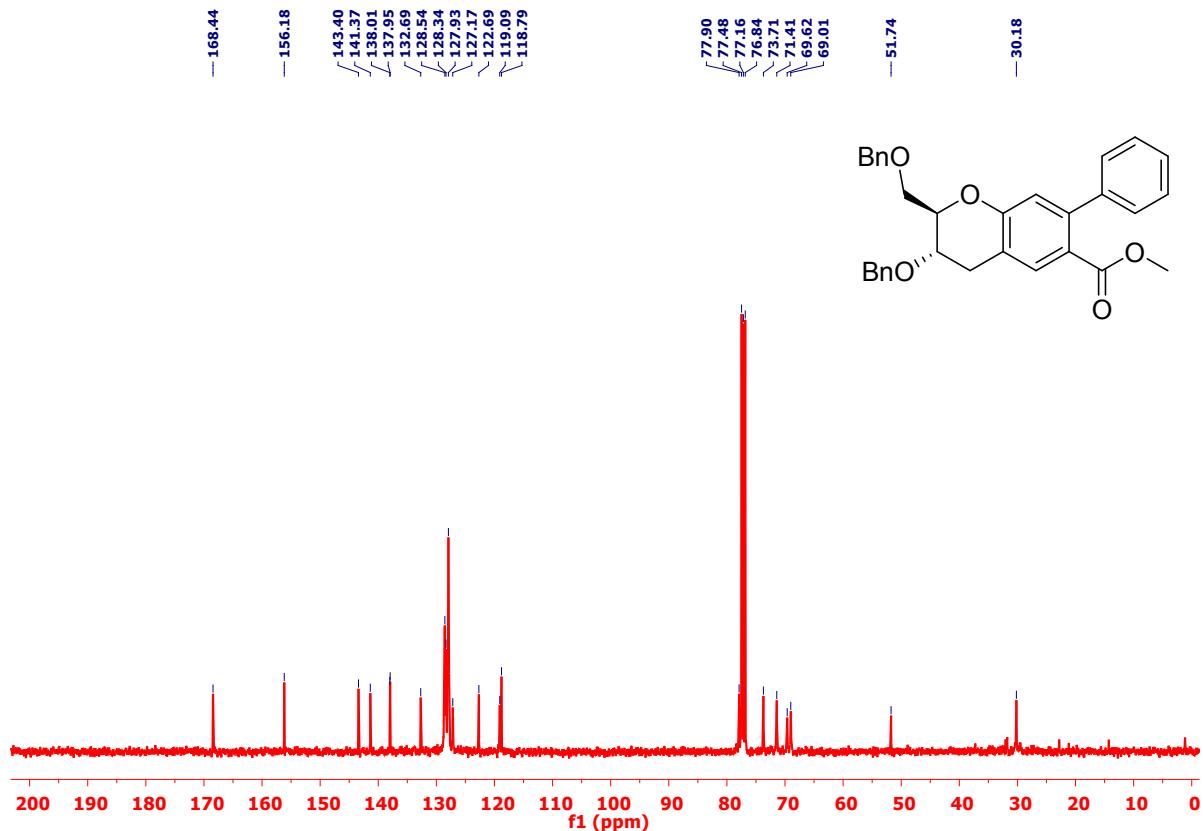


Figure S45. ¹³C NMR spectrum of compound **5h** (100.6 MHz, CDCl₃)

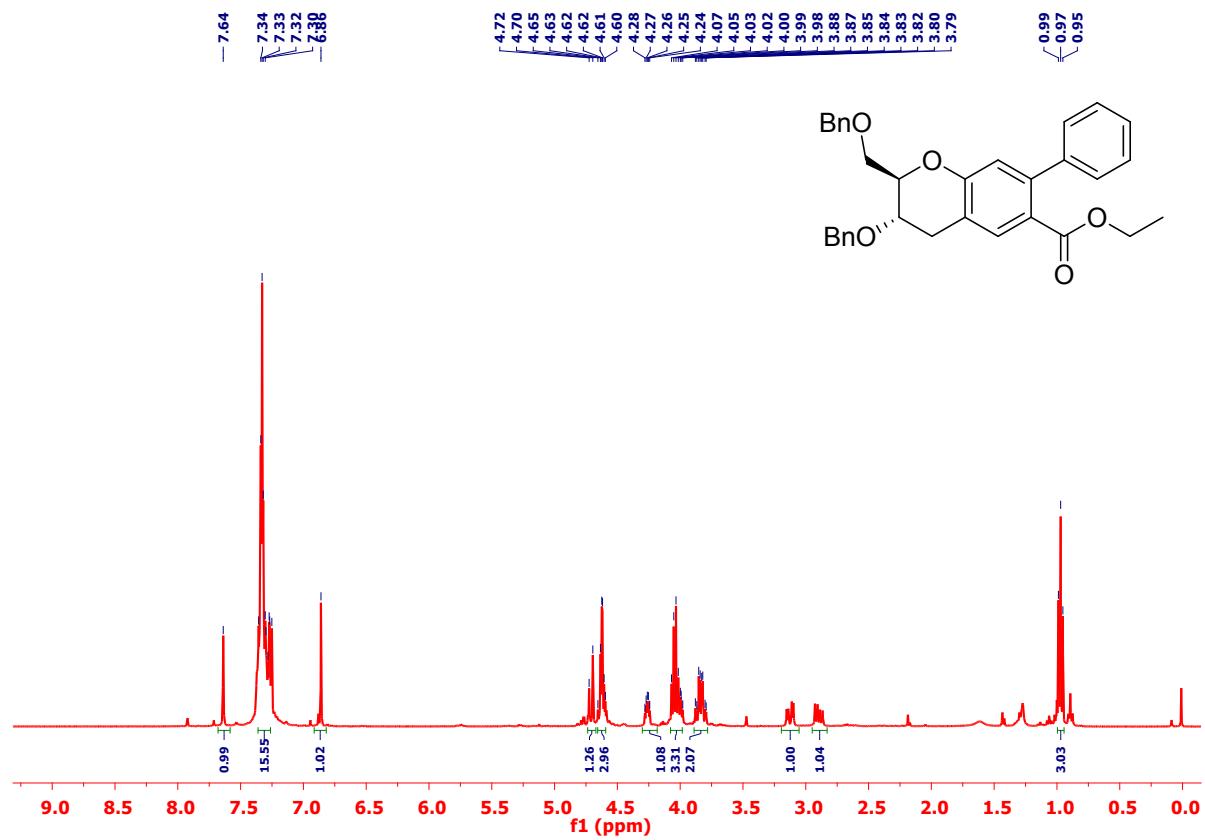


Figure S46. ¹H NMR spectrum of compound **5i** (400 MHz, CDCl₃)

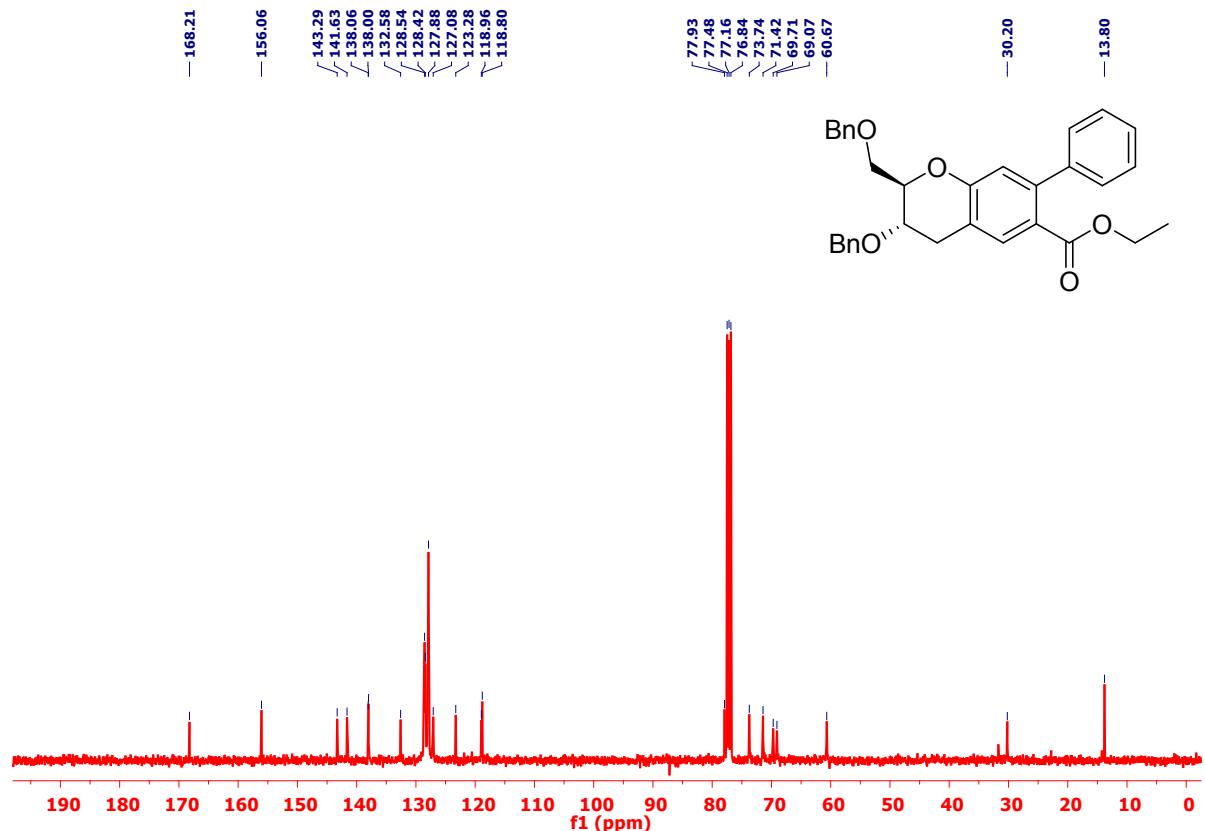


Figure S47. ¹³C NMR spectrum of compound **5i** (100.6 MHz, CDCl₃)

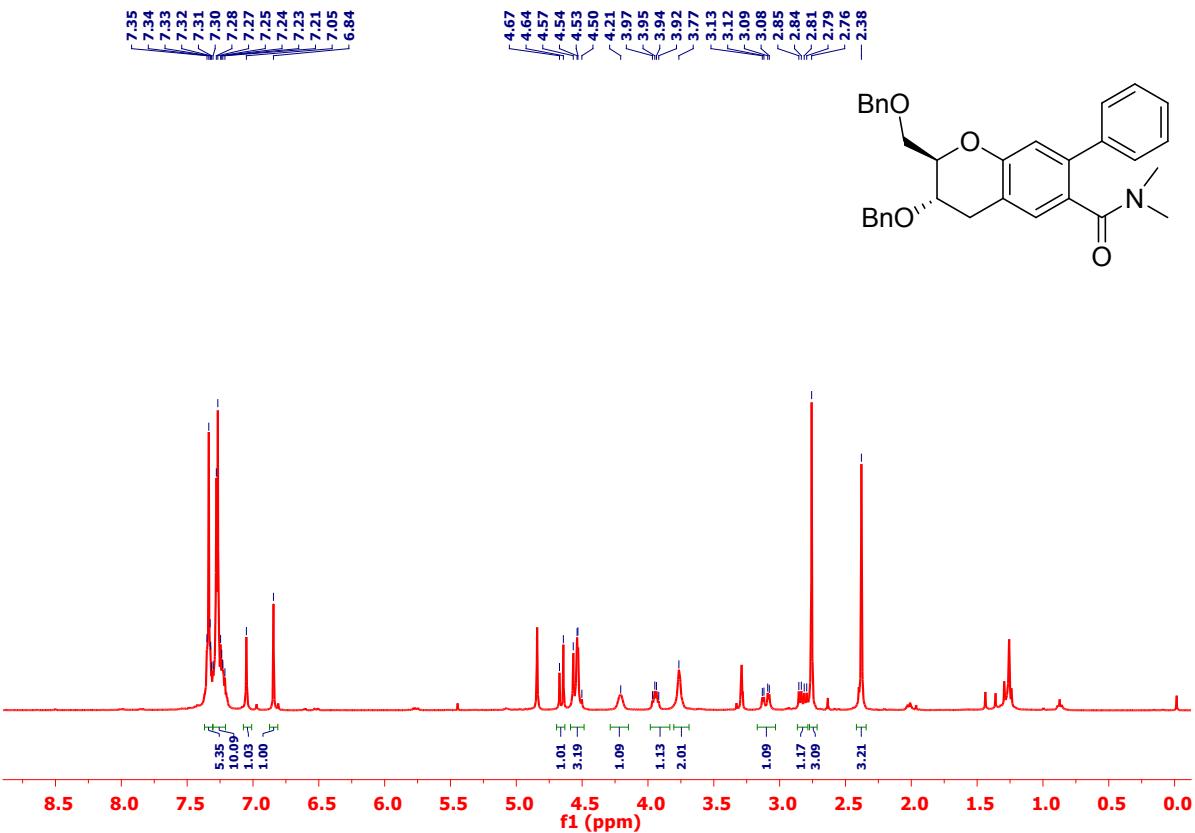


Figure S48. ¹H NMR spectrum of compound **5j** (400 MHz, CD₃OD)

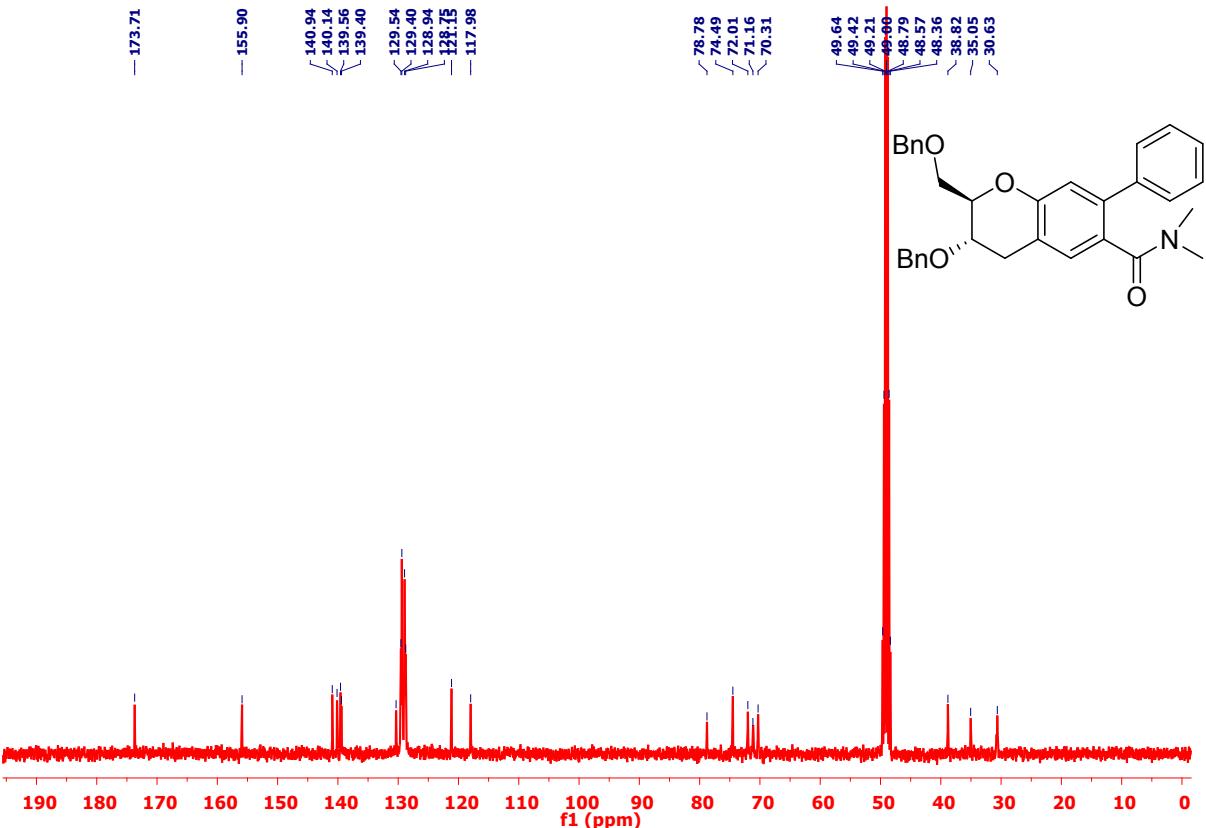


Figure S49. ¹³C NMR spectrum of compound **5j** (100.6 MHz, CD₃OD)

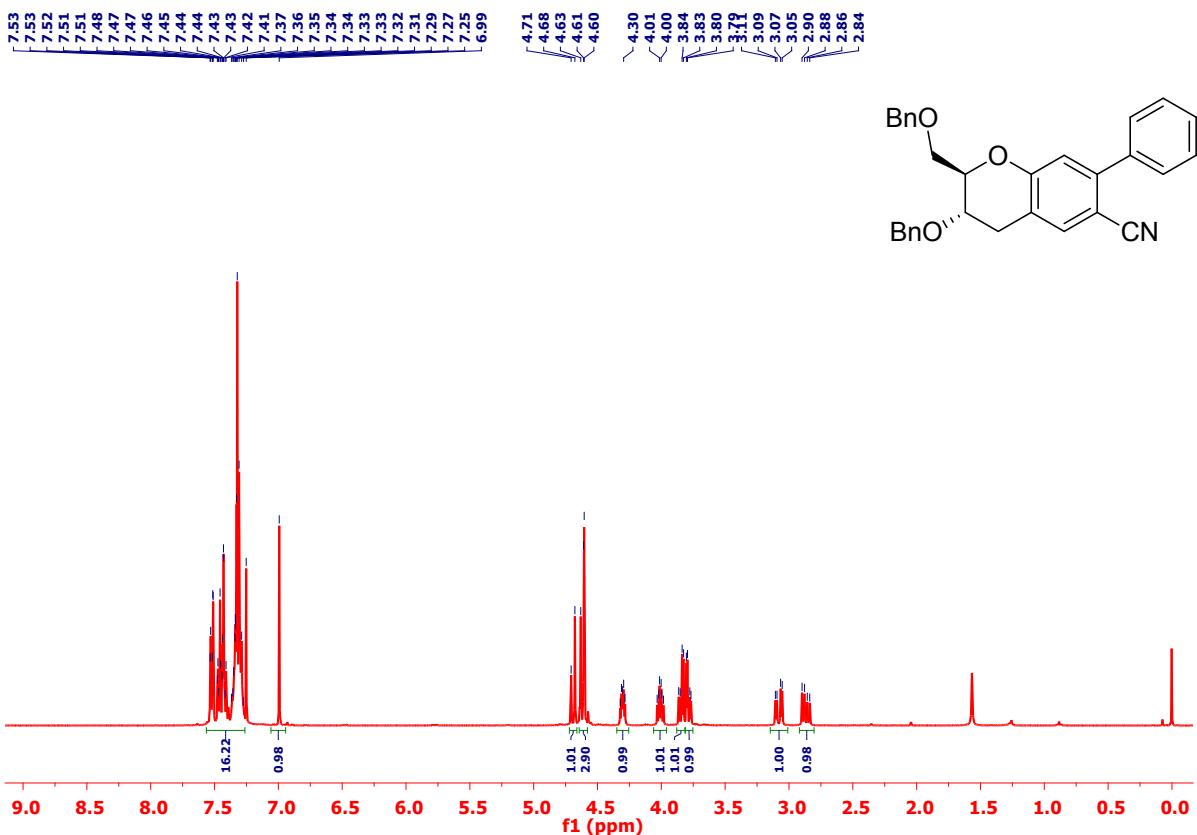


Figure S50. ¹H NMR spectrum of compound **5k** (400 MHz, CDCl₃)

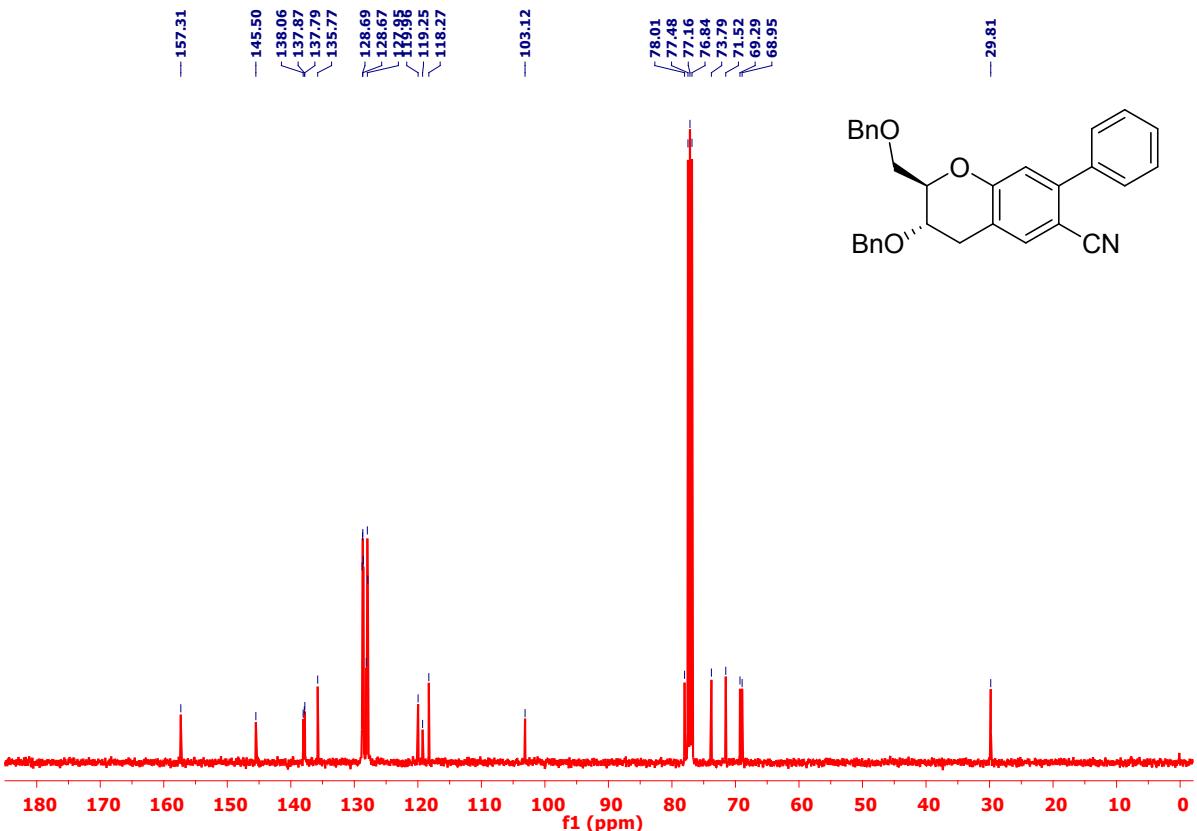


Figure S51. ¹³C NMR spectrum of compound **5k** (100.6 MHz, CDCl₃)

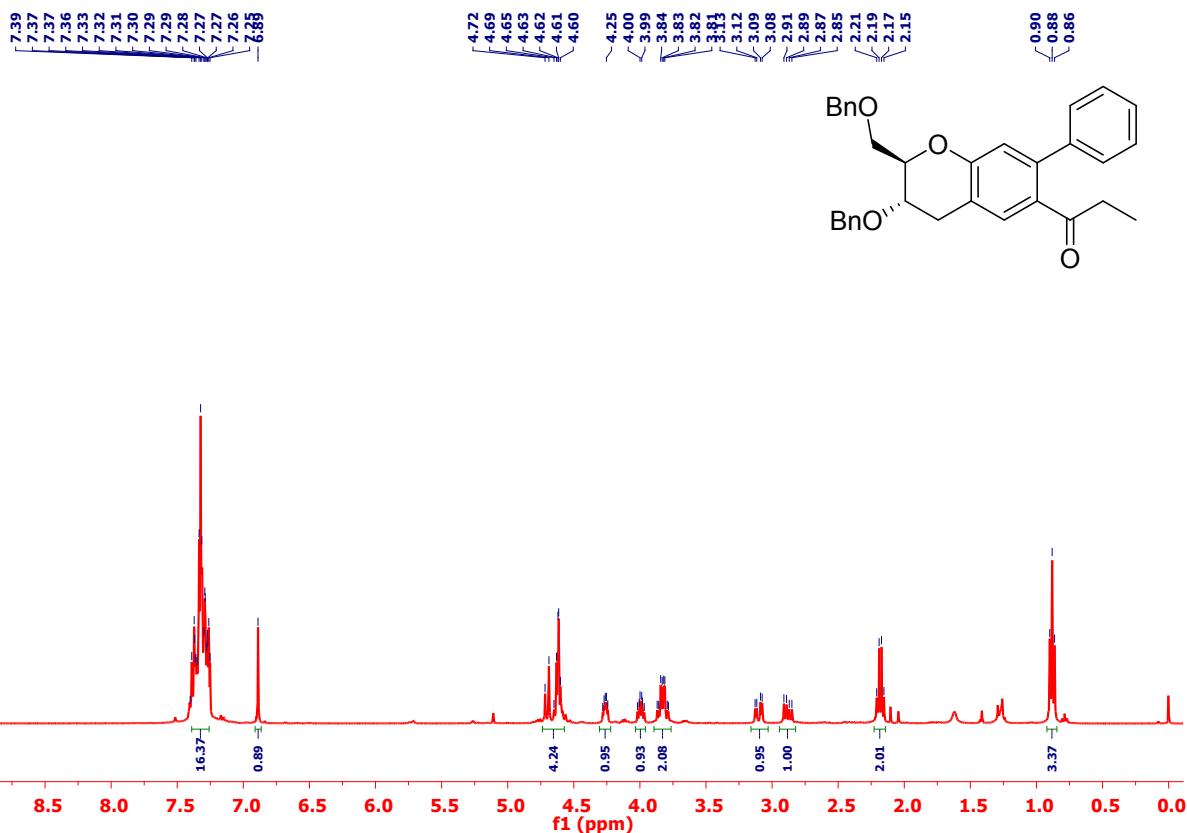


Figure S52. ¹H NMR spectrum of compound **5l** (400 MHz, CDCl₃)

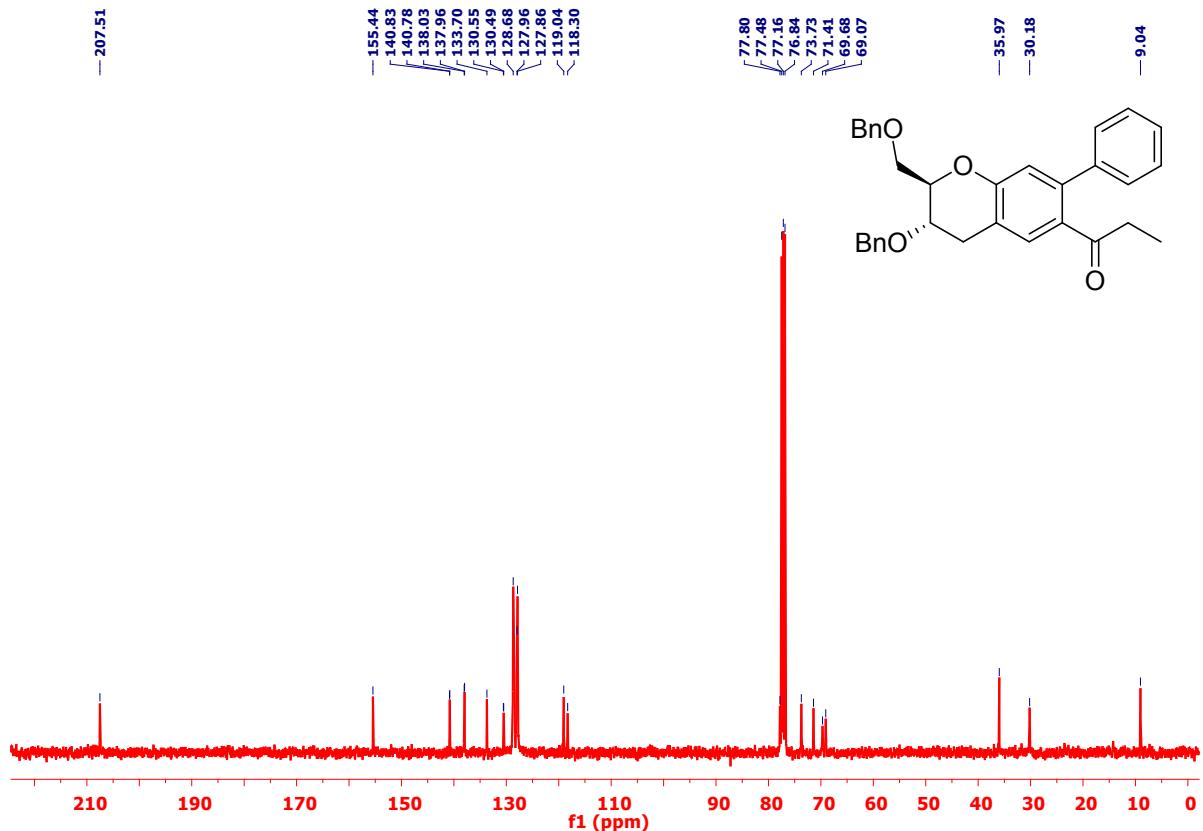


Figure S53. ¹³C NMR spectrum of compound **5l** (100.6 MHz, CDCl₃)

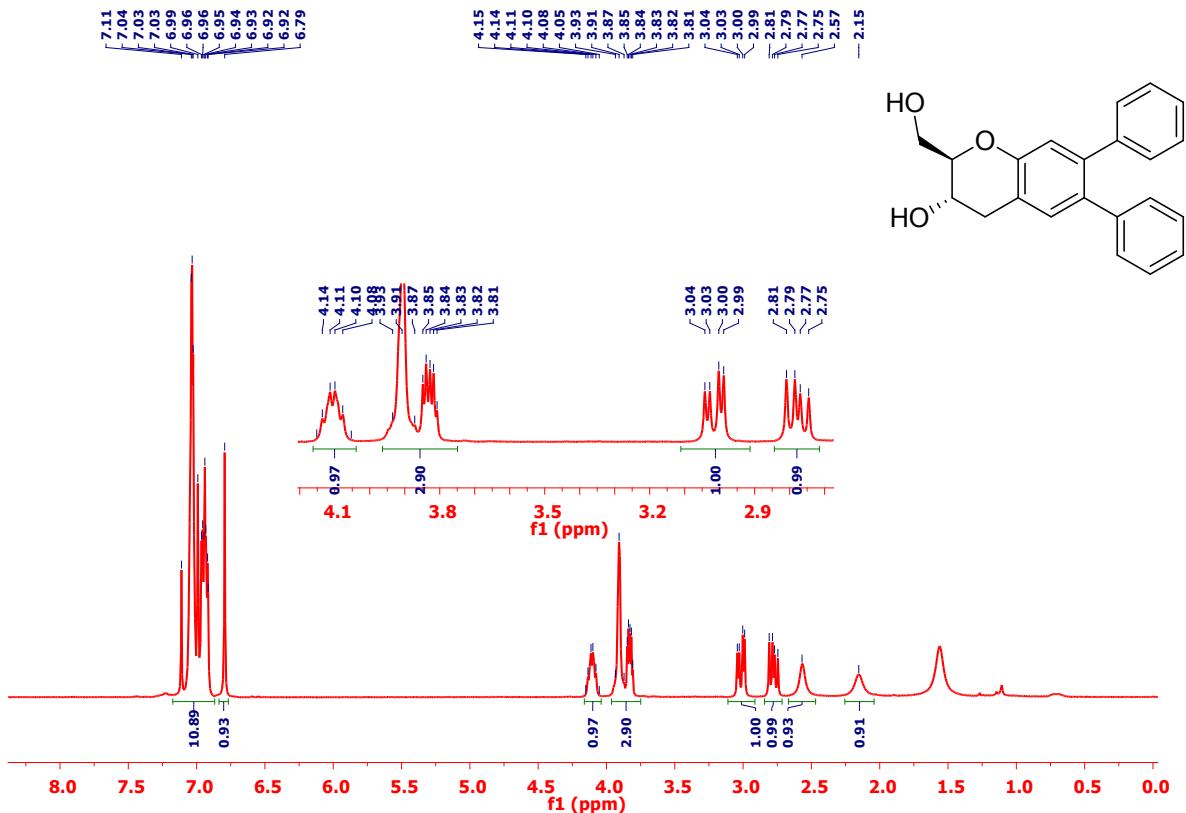


Figure S54. ^1H NMR spectrum of compound **6a** (400 MHz, CDCl_3)

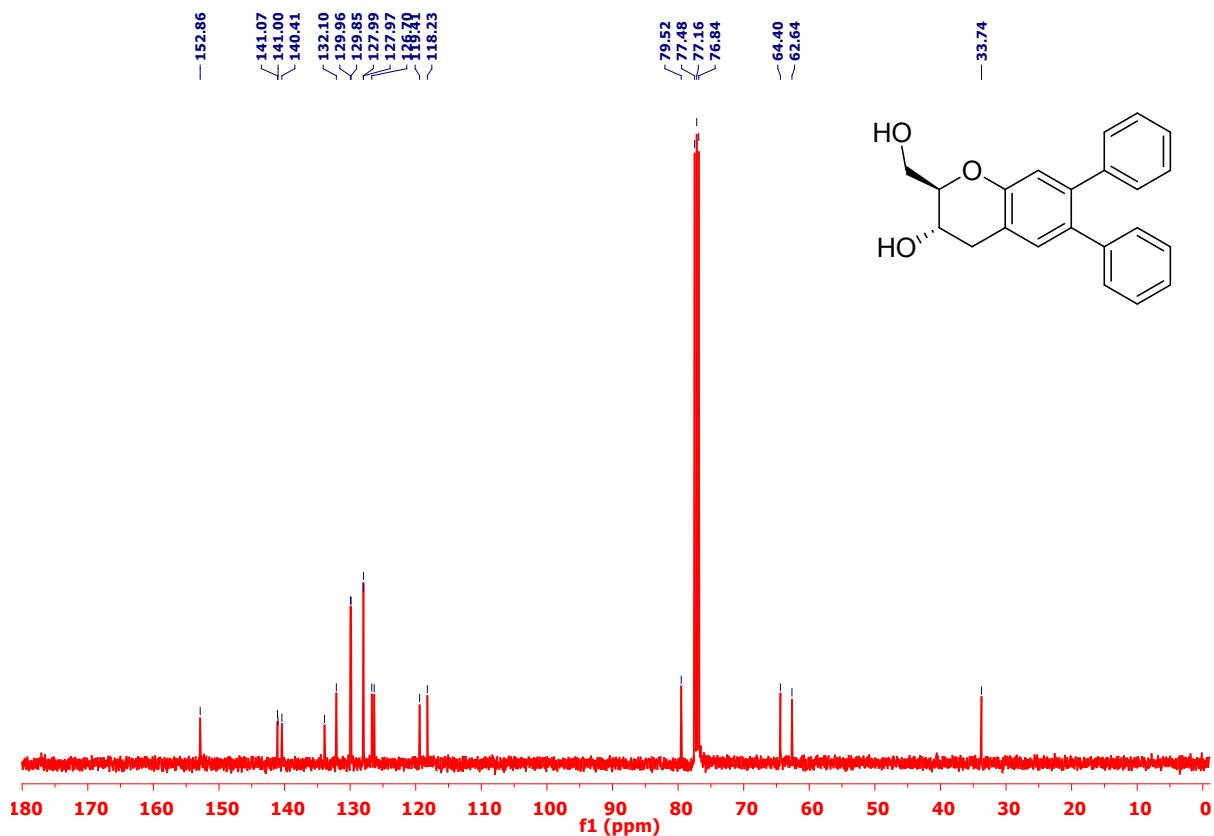


Figure S55. ^{13}C NMR spectrum of compound **6a** (100.6 MHz, CDCl_3)

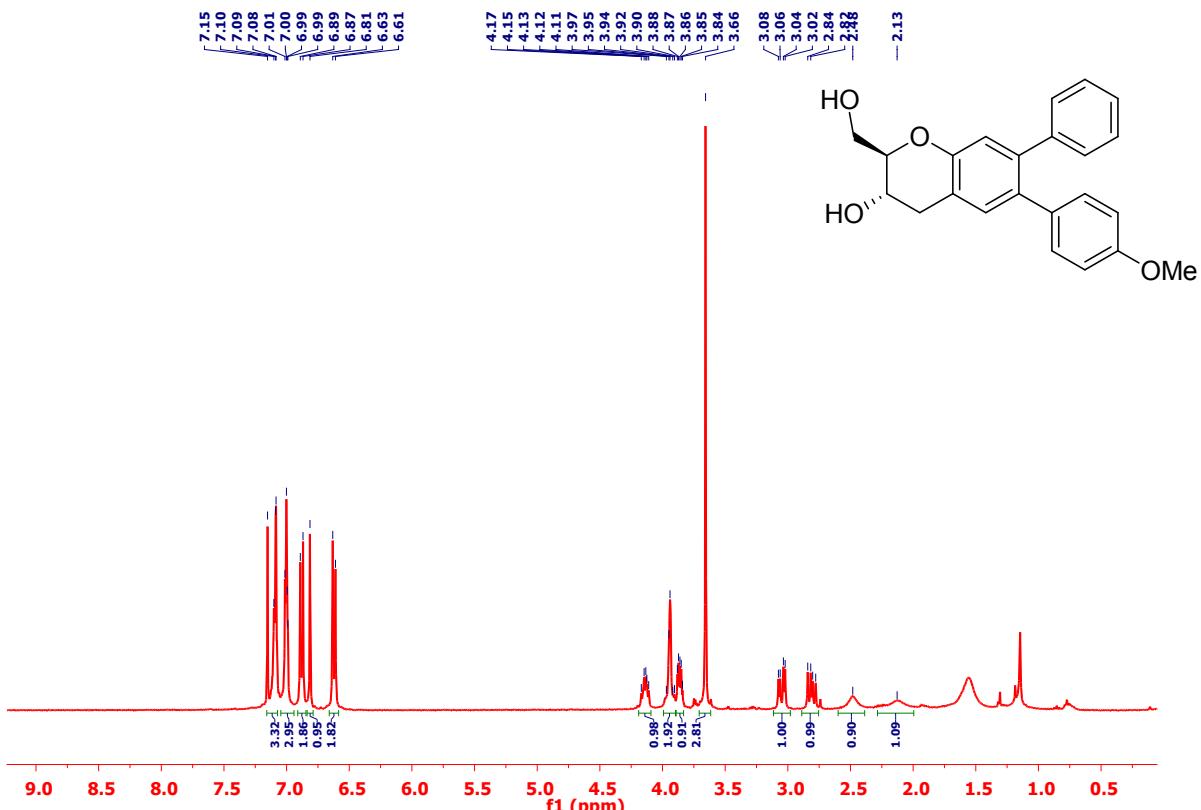


Figure S56. ¹H NMR spectrum of compound **6d** (400 MHz, CDCl₃)

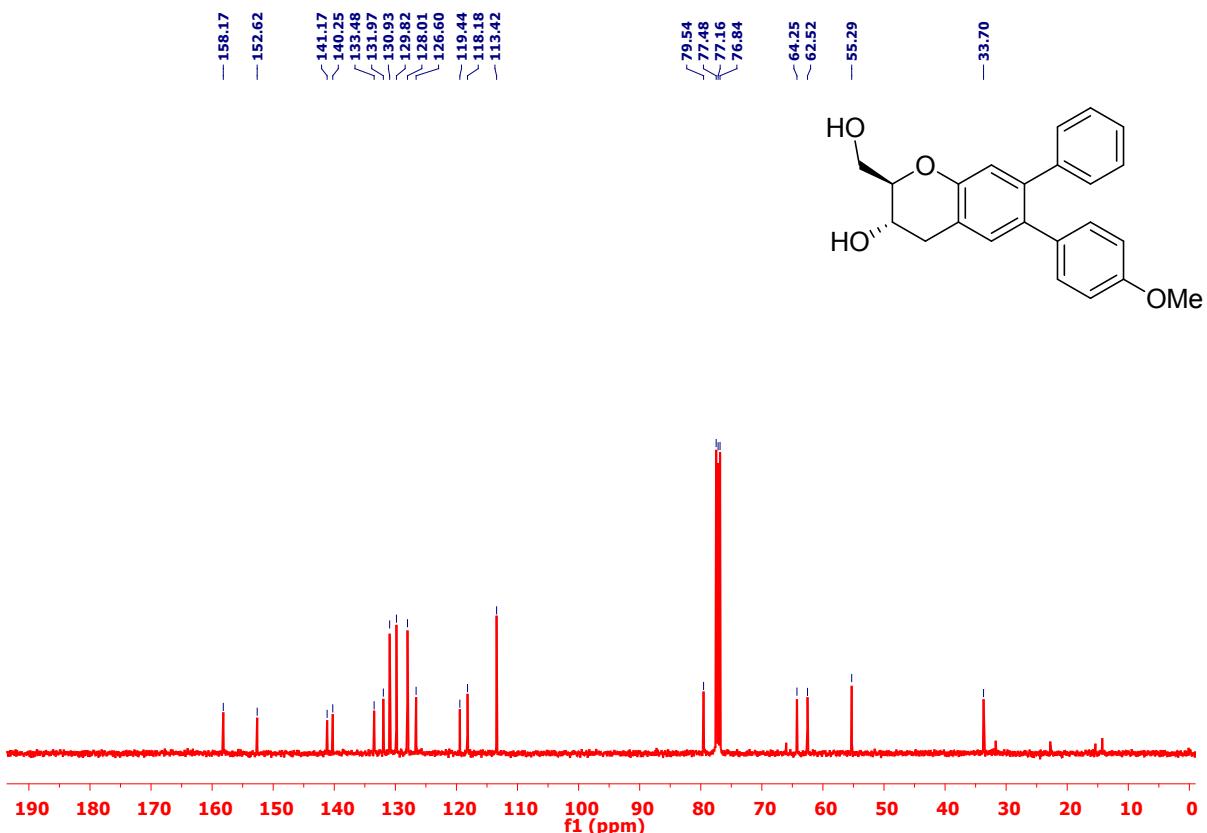


Figure S57. ¹³C NMR spectrum of compound **6d** (100.6 MHz, CDCl₃)

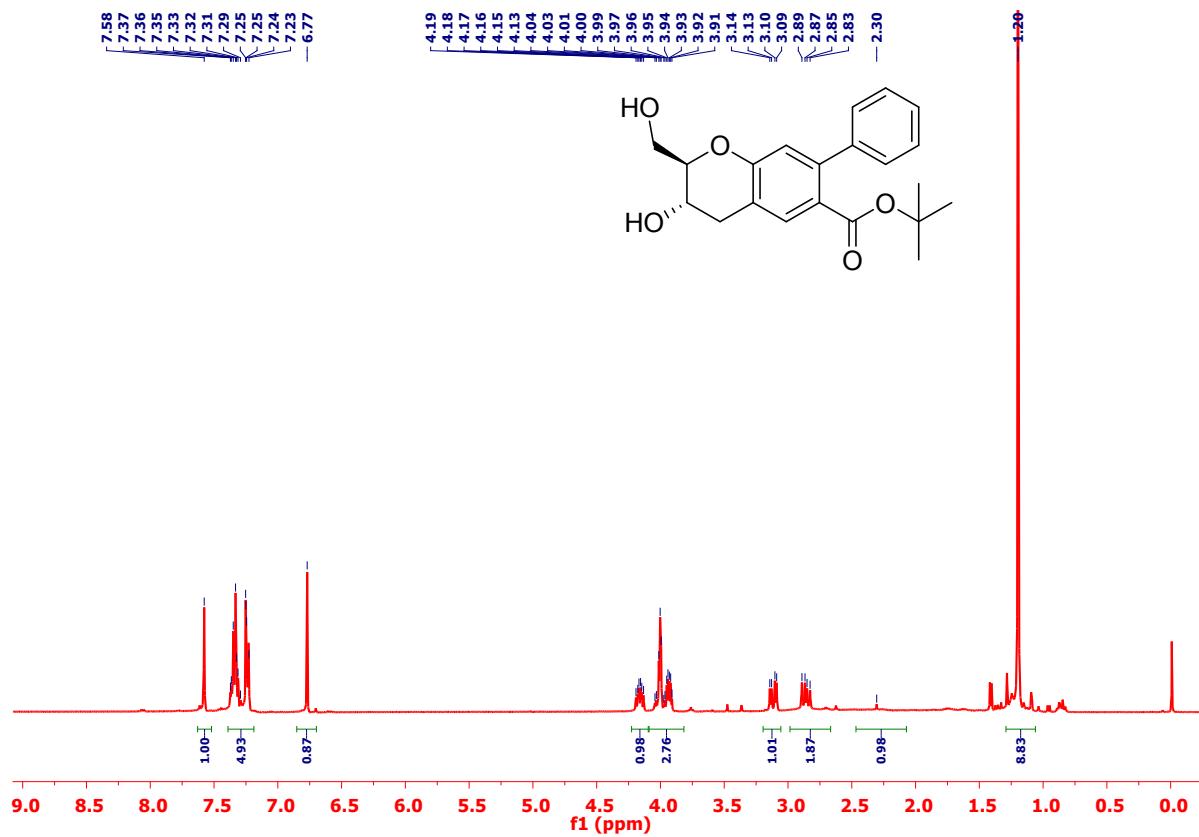


Figure S58. ¹H NMR spectrum of compound **6e** (400 MHz, CDCl₃)

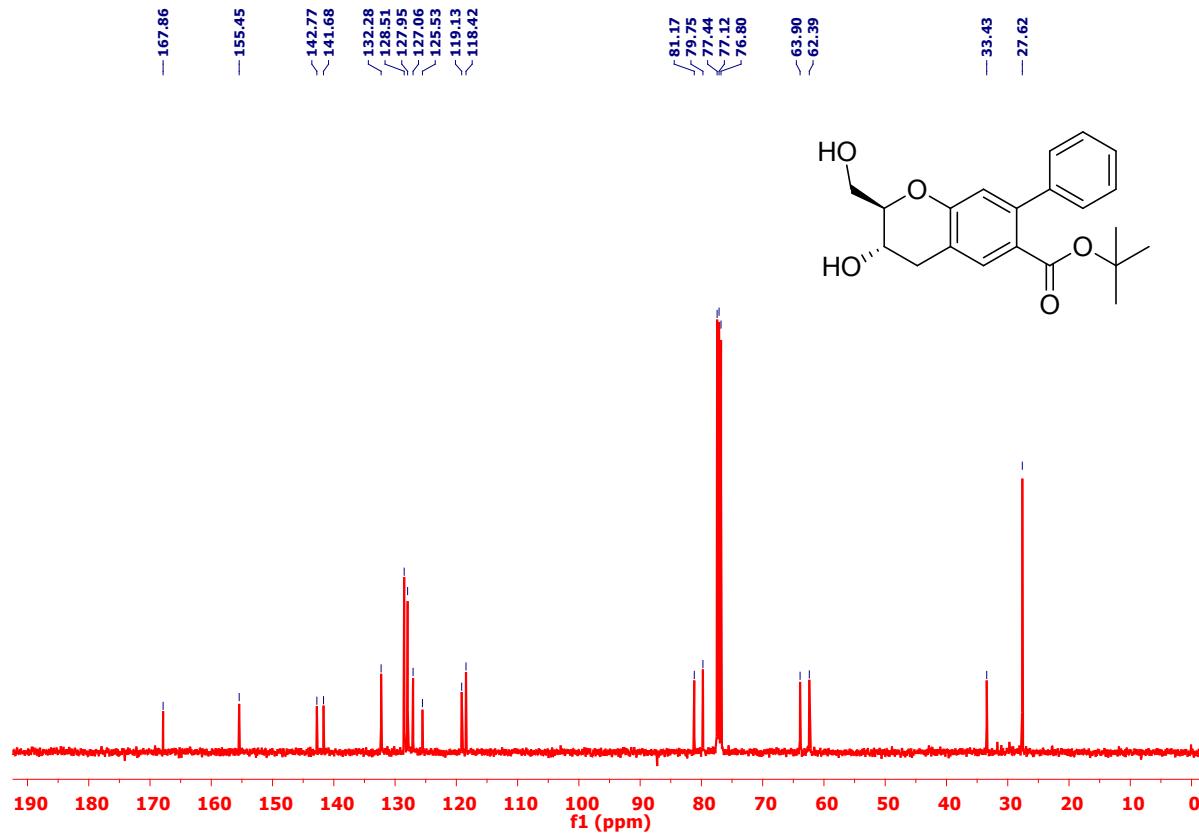


Figure S59. ¹³C NMR spectrum of compound **6e** (100.6 MHz, CDCl₃)

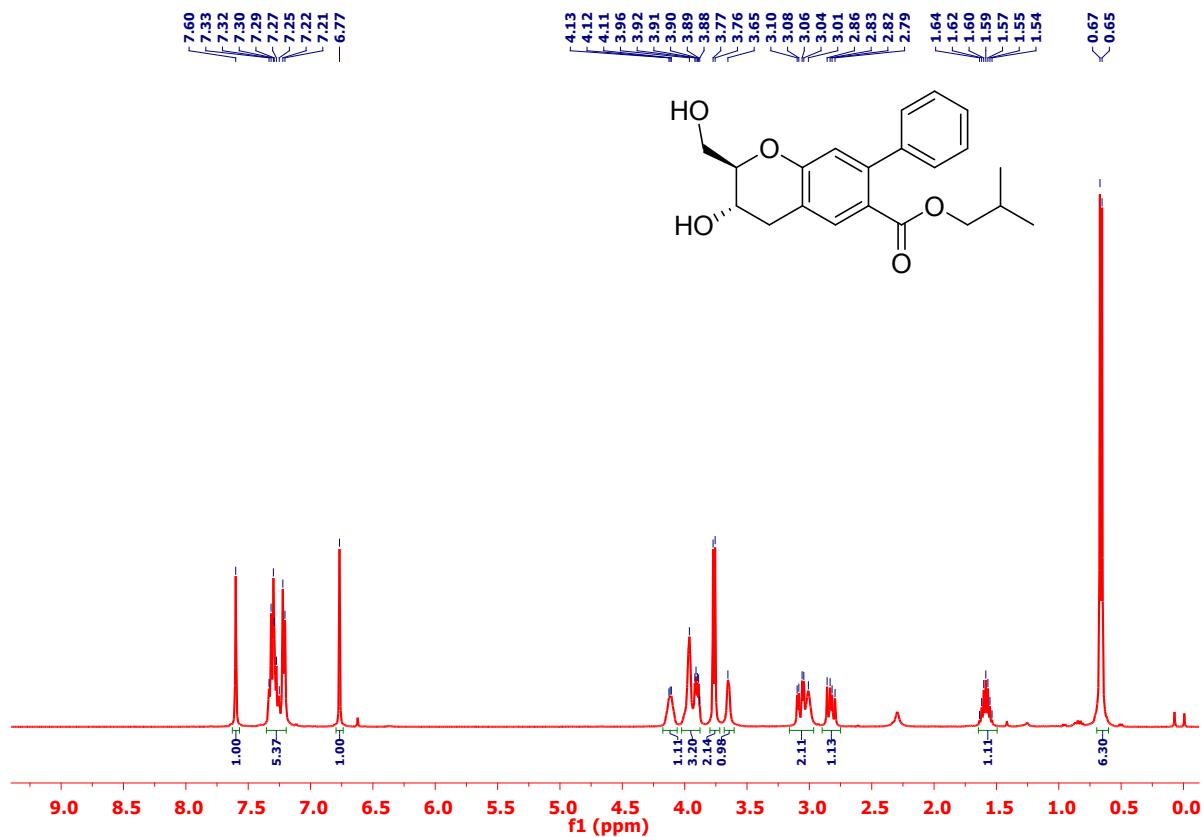


Figure S60. ¹H NMR spectrum of compound **6f** (400 MHz, CDCl₃)

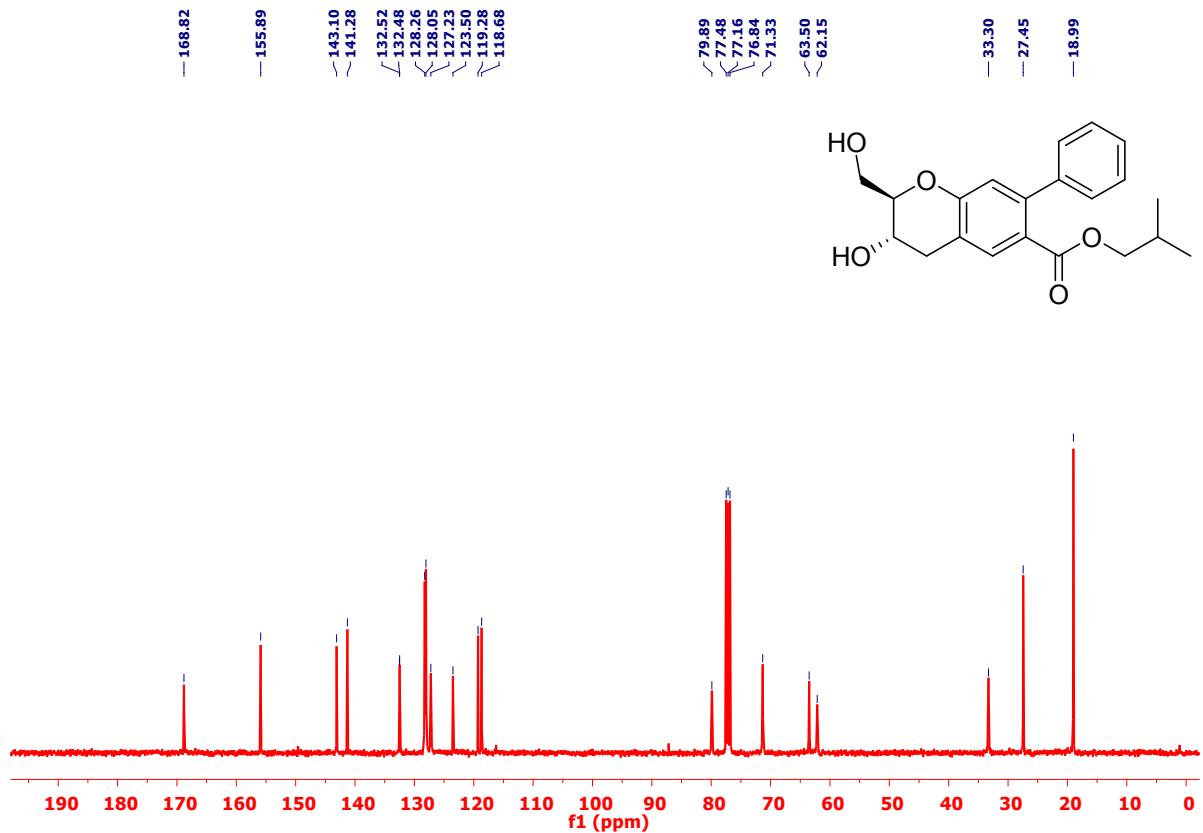


Figure S61. ¹³C NMR spectrum of compound **6f** (100.6 MHz, CDCl₃)

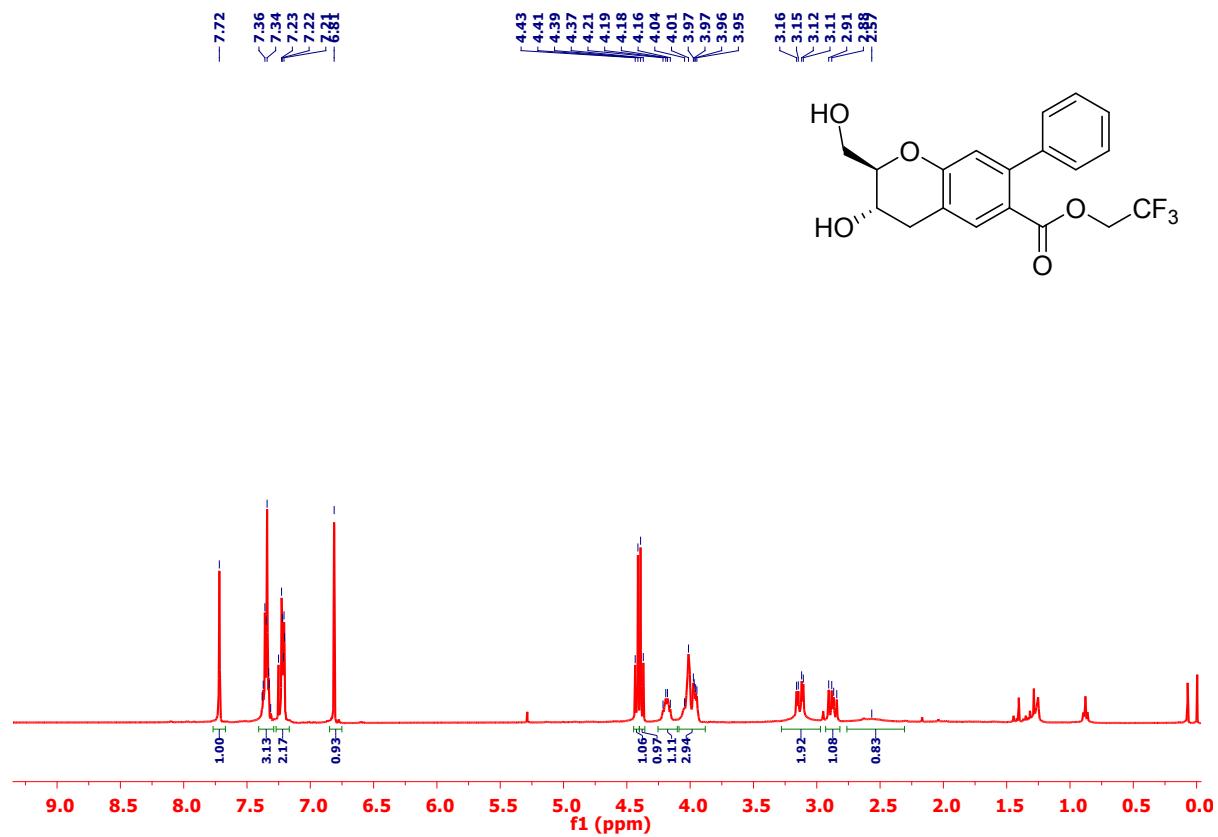


Figure S62. ¹H NMR spectrum of compound **6g** (400 MHz, CDCl₃)

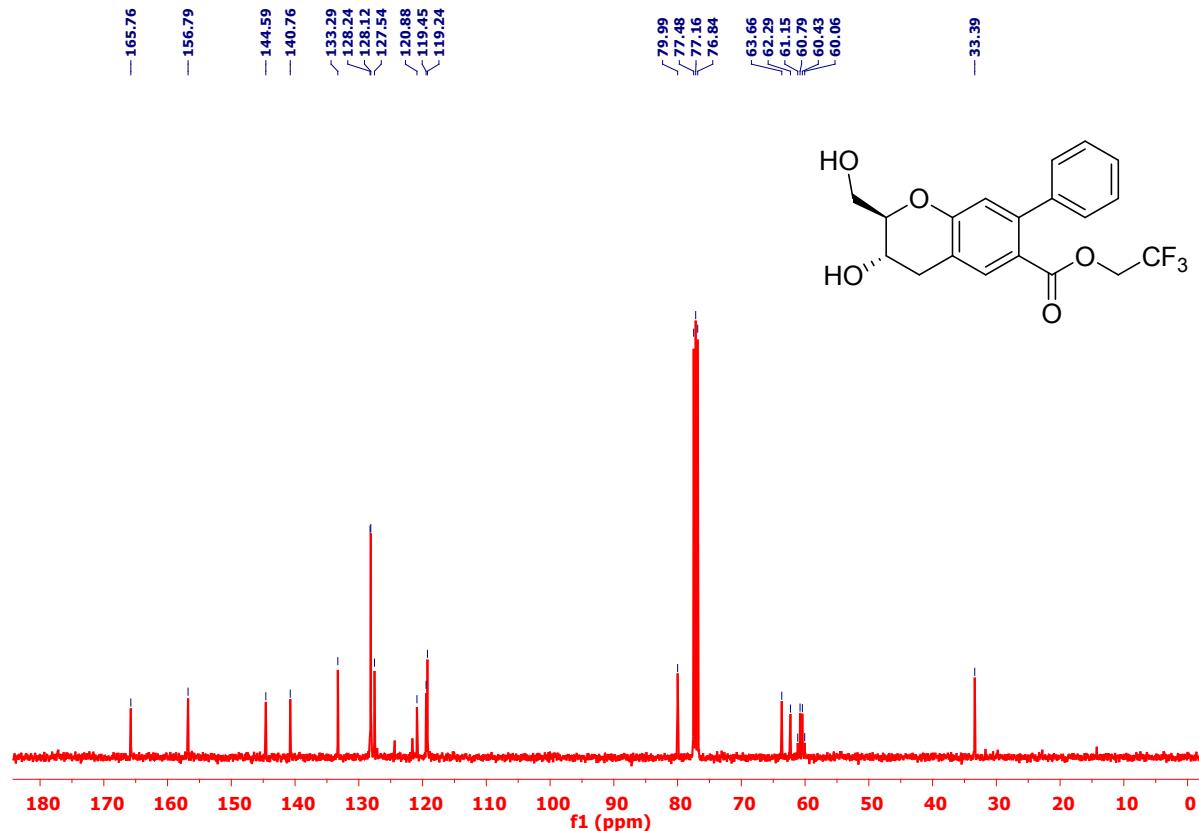


Figure S63. ¹³C NMR spectrum of compound **6g** (100.6 MHz, CDCl₃)

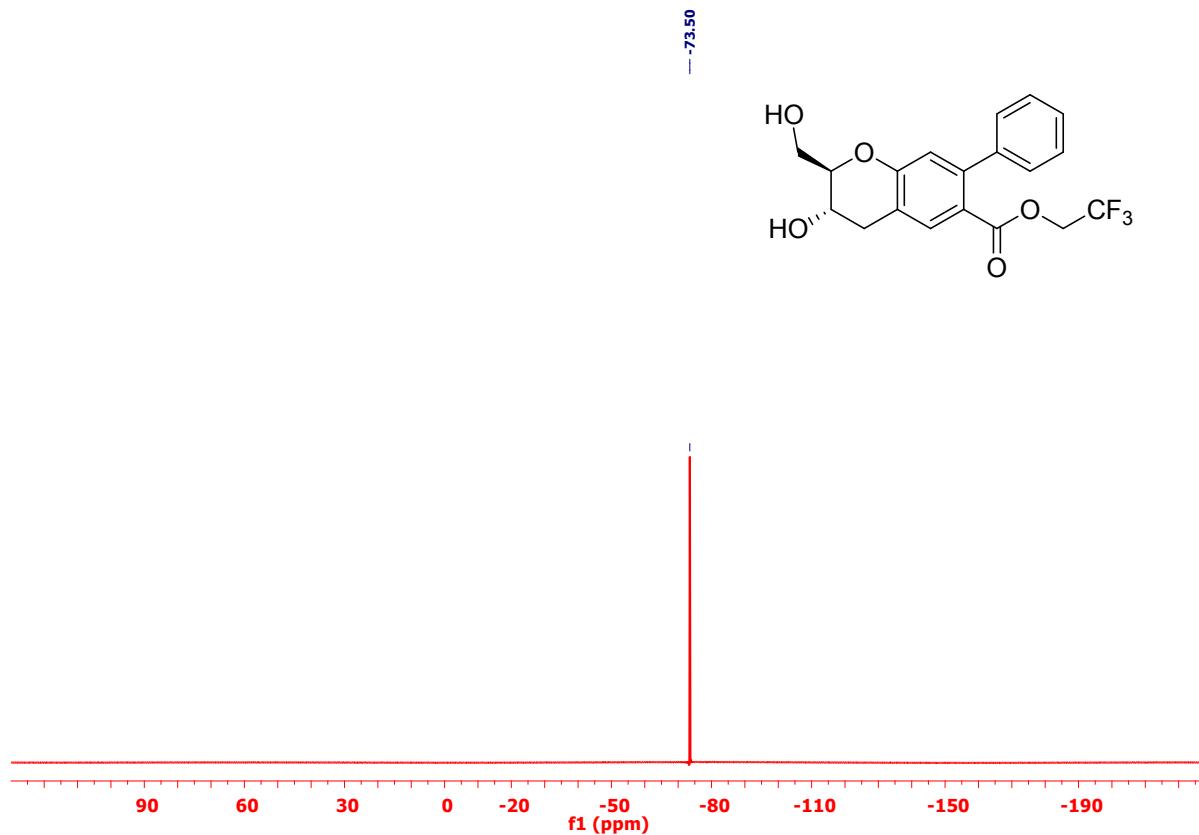


Figure S64. ^{19}F NMR spectrum of compound **6g** (376 MHz, CDCl_3)

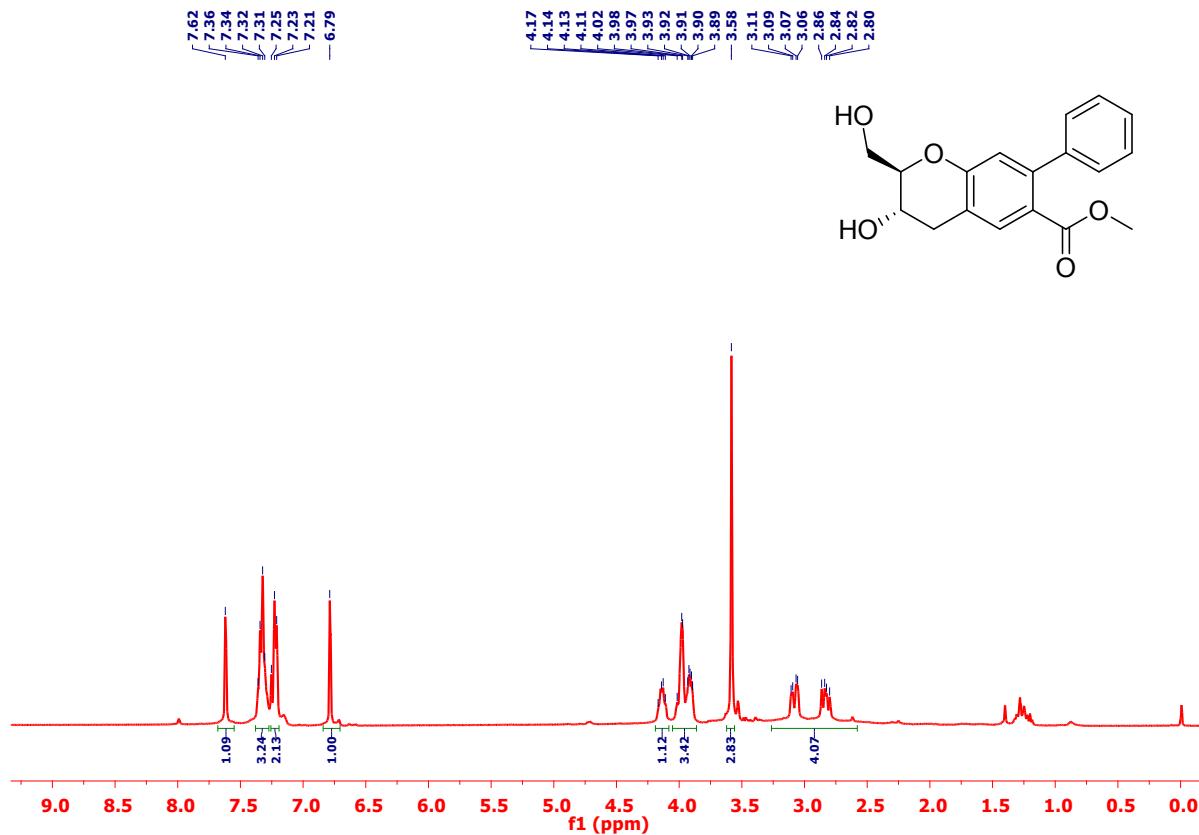


Figure S65. ¹H NMR spectrum of compound **6h** (400 MHz, CDCl₃)

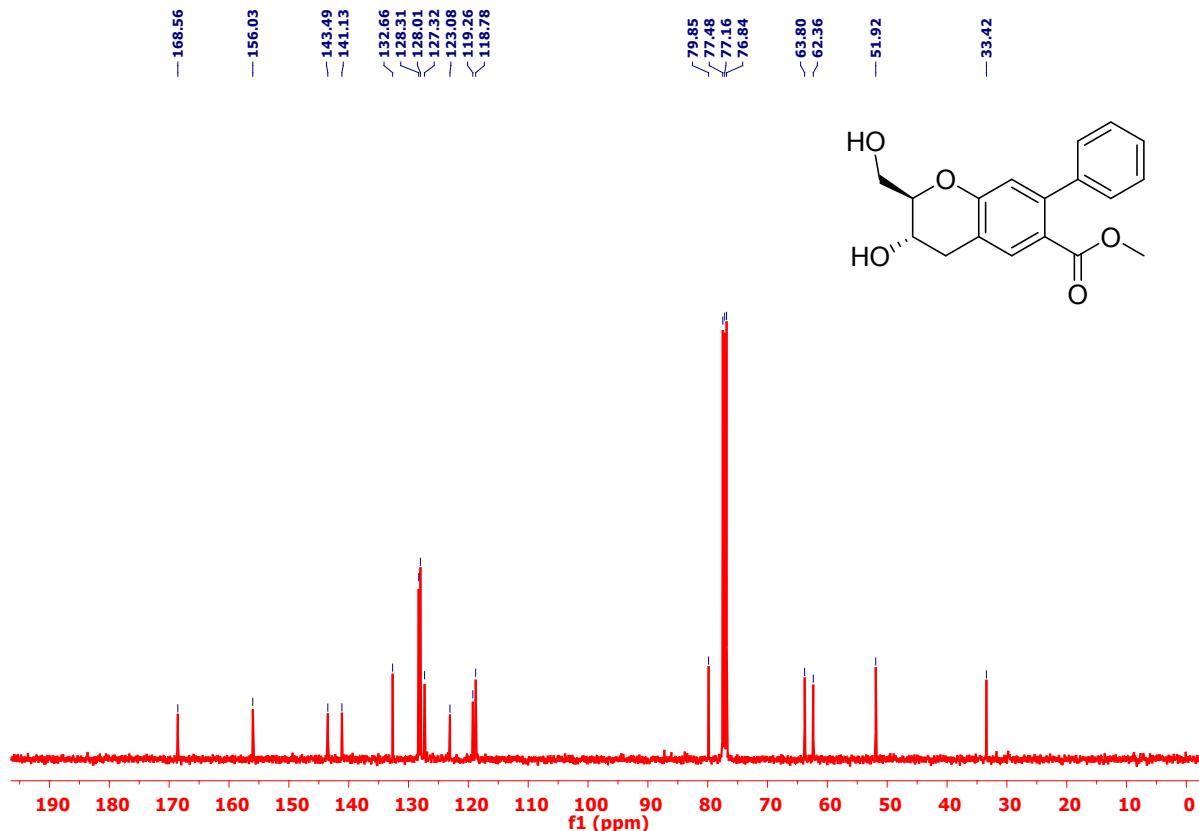


Figure S66. ¹³C NMR spectrum of compound **6h** (100.6 MHz, CDCl₃)

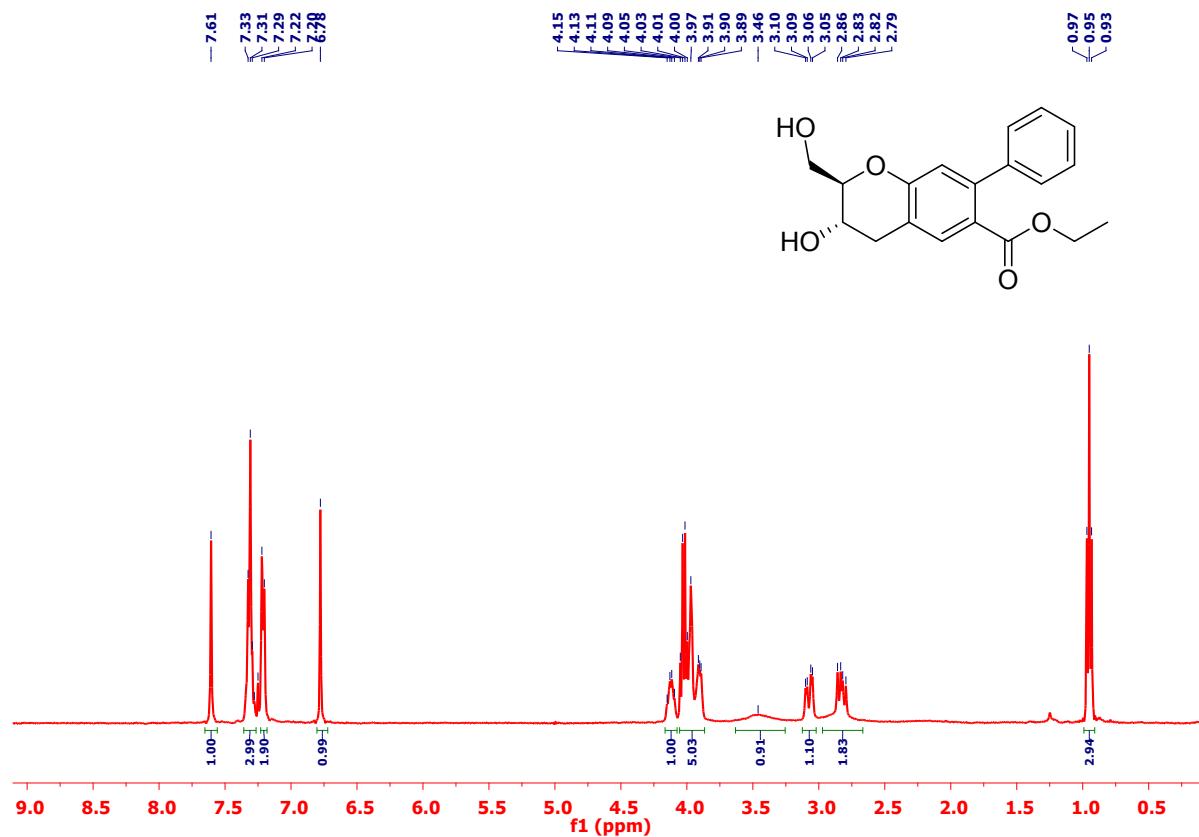


Figure S67. ¹H NMR spectrum of compound **6i** (400 MHz, CDCl₃)

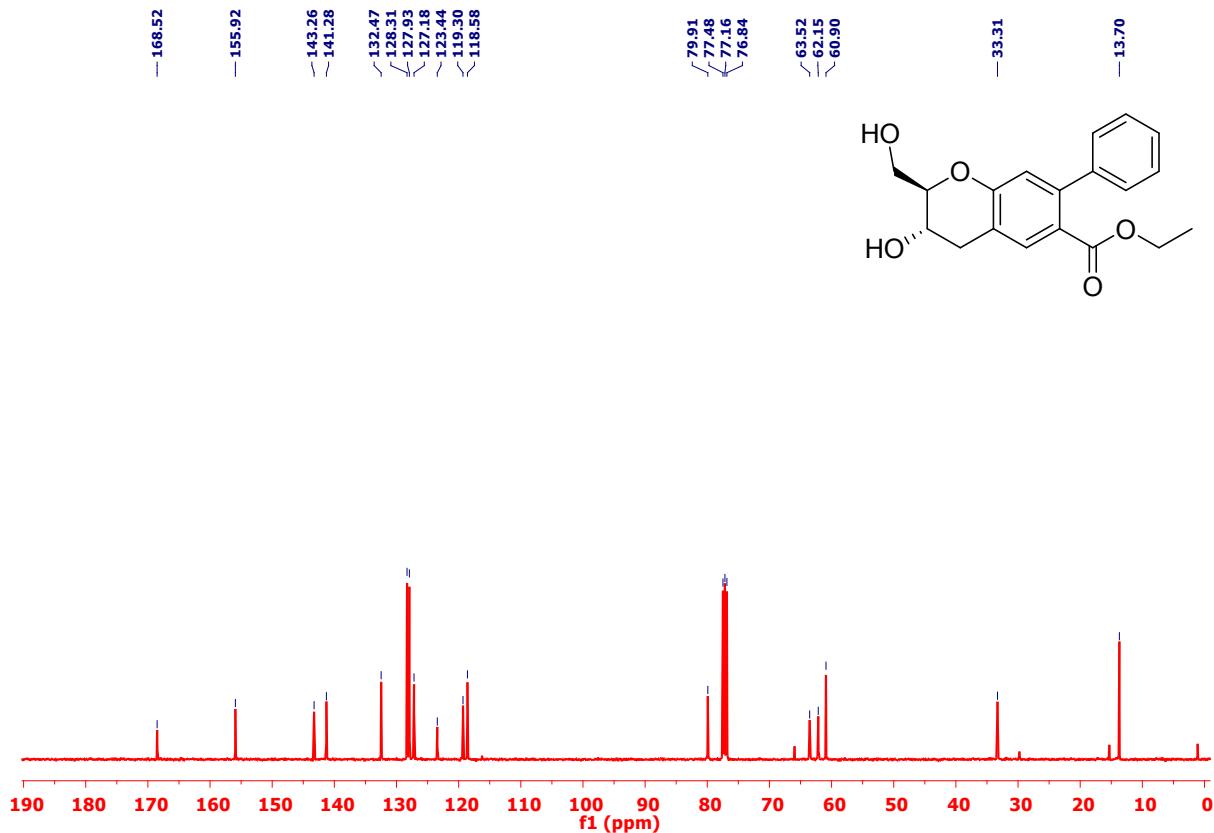


Figure S68. ¹³C NMR spectrum of compound **6i** (100.6 MHz, CDCl₃)

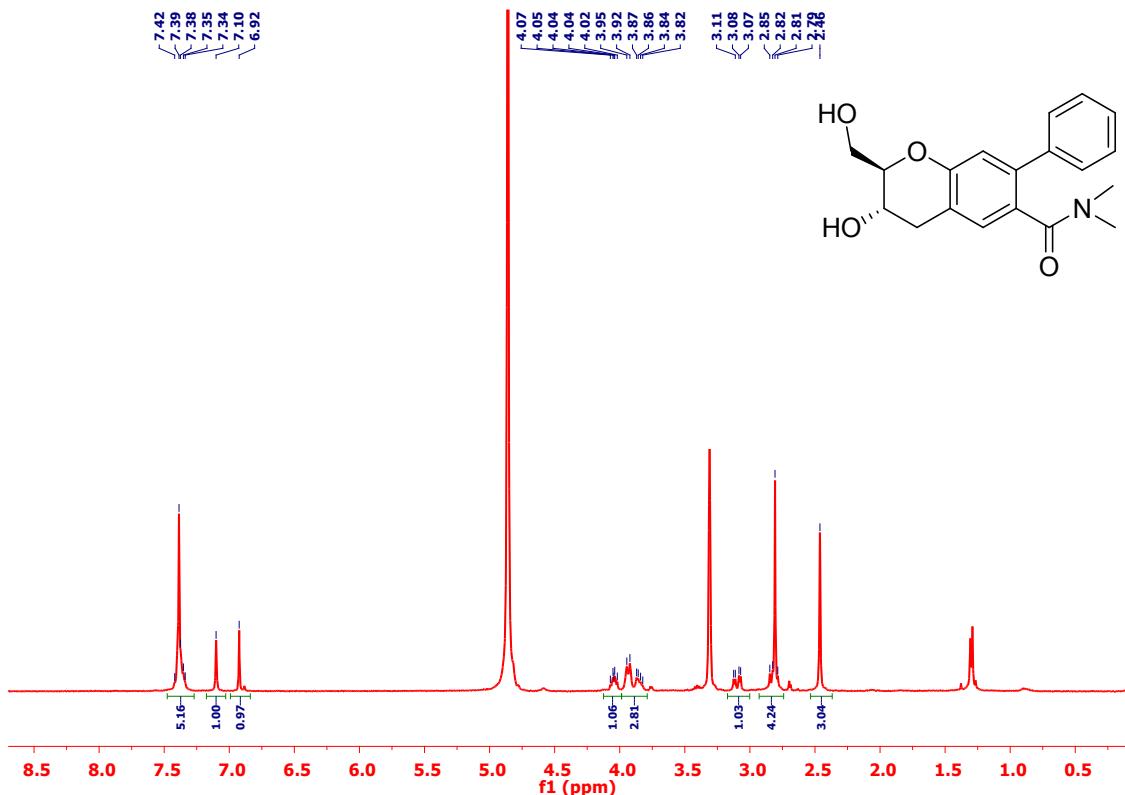


Figure S69. ¹H NMR spectrum of compound 6j (400 MHz, CD₃OD)

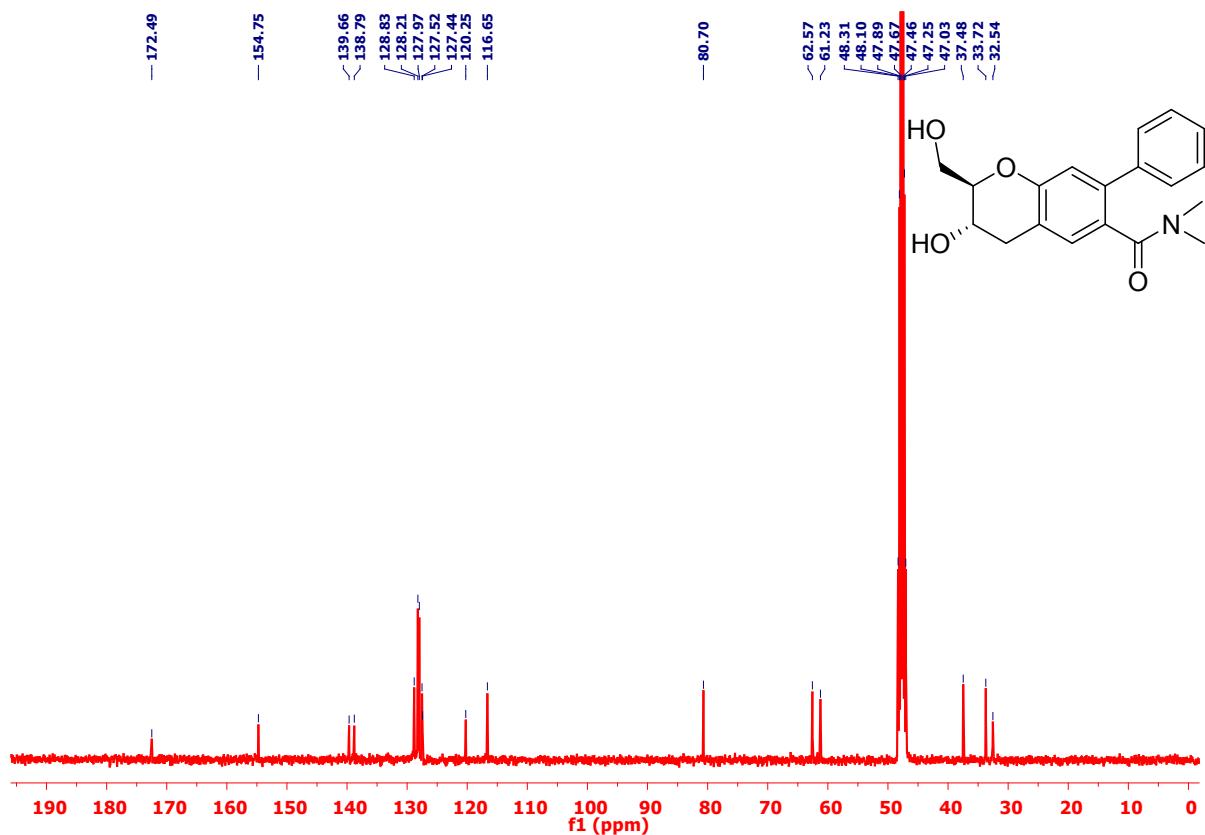


Figure S70. ¹³C NMR spectrum of compound 6j (100.6 MHz, CD₃OD)

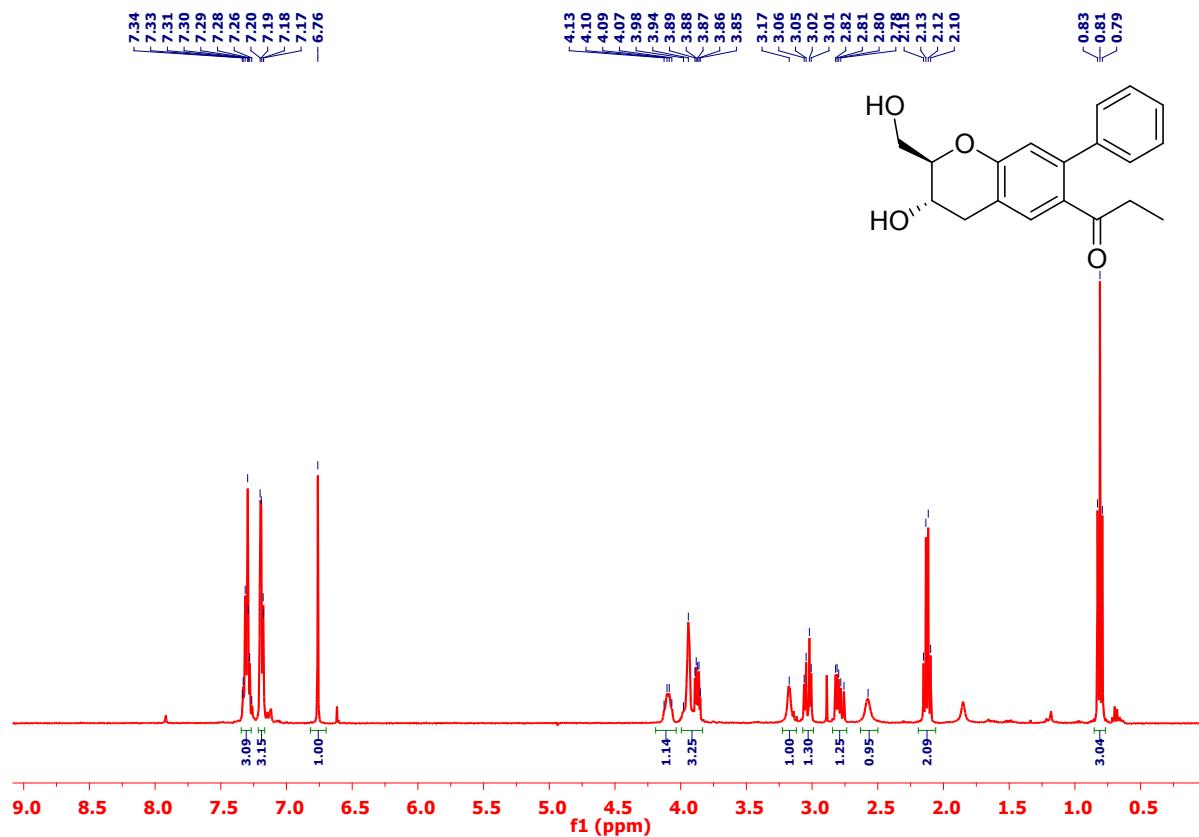


Figure S71. ¹H NMR spectrum of compound **6l** (400 MHz, CDCl₃)

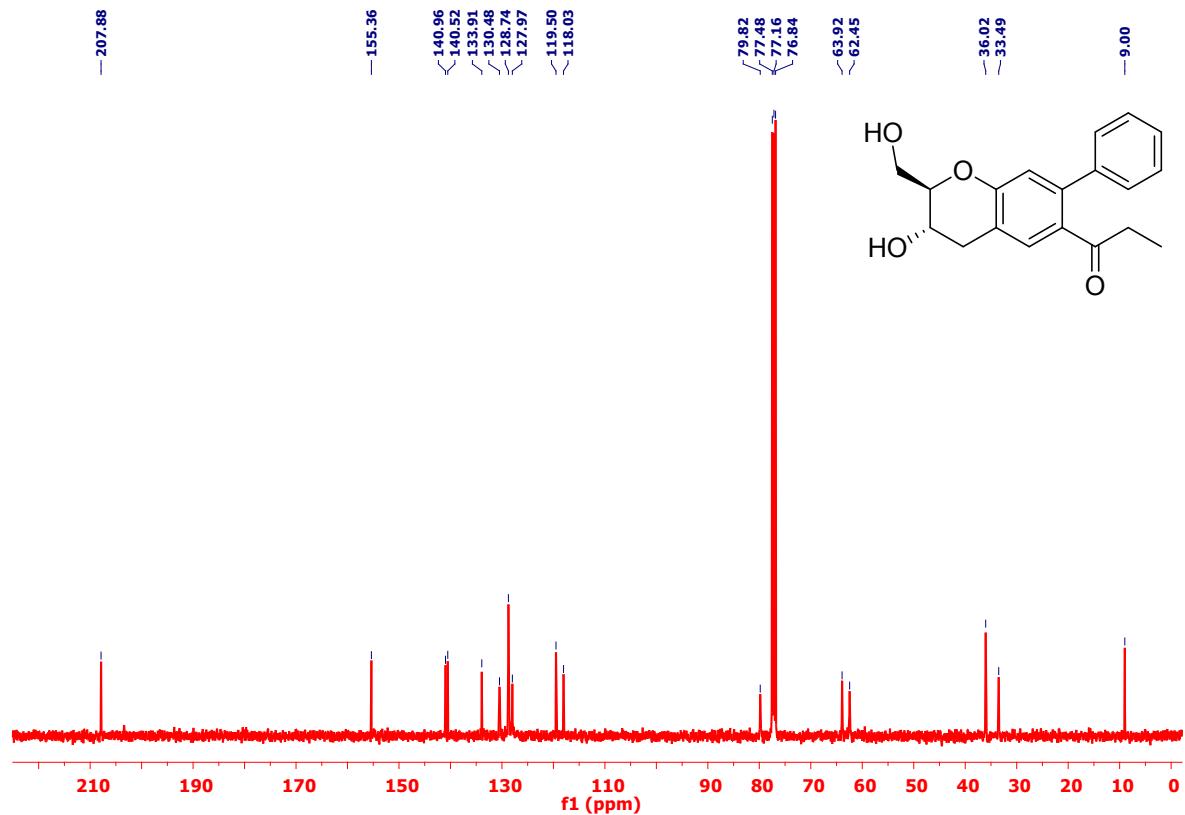


Figure S72. ¹³C NMR spectrum of compound **6l** (100.6 MHz, CDCl₃)

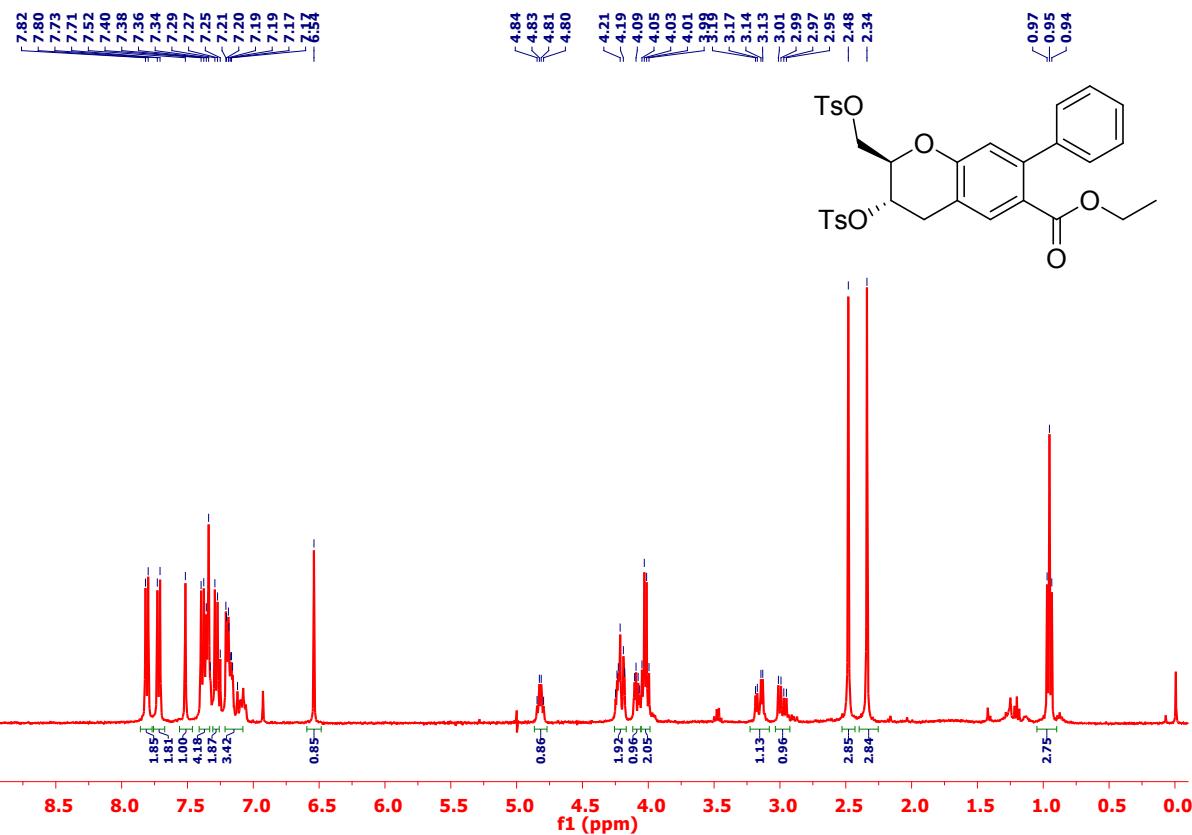


Figure S73. ¹H NMR spectrum of compound 7 (400 MHz, CDCl₃)

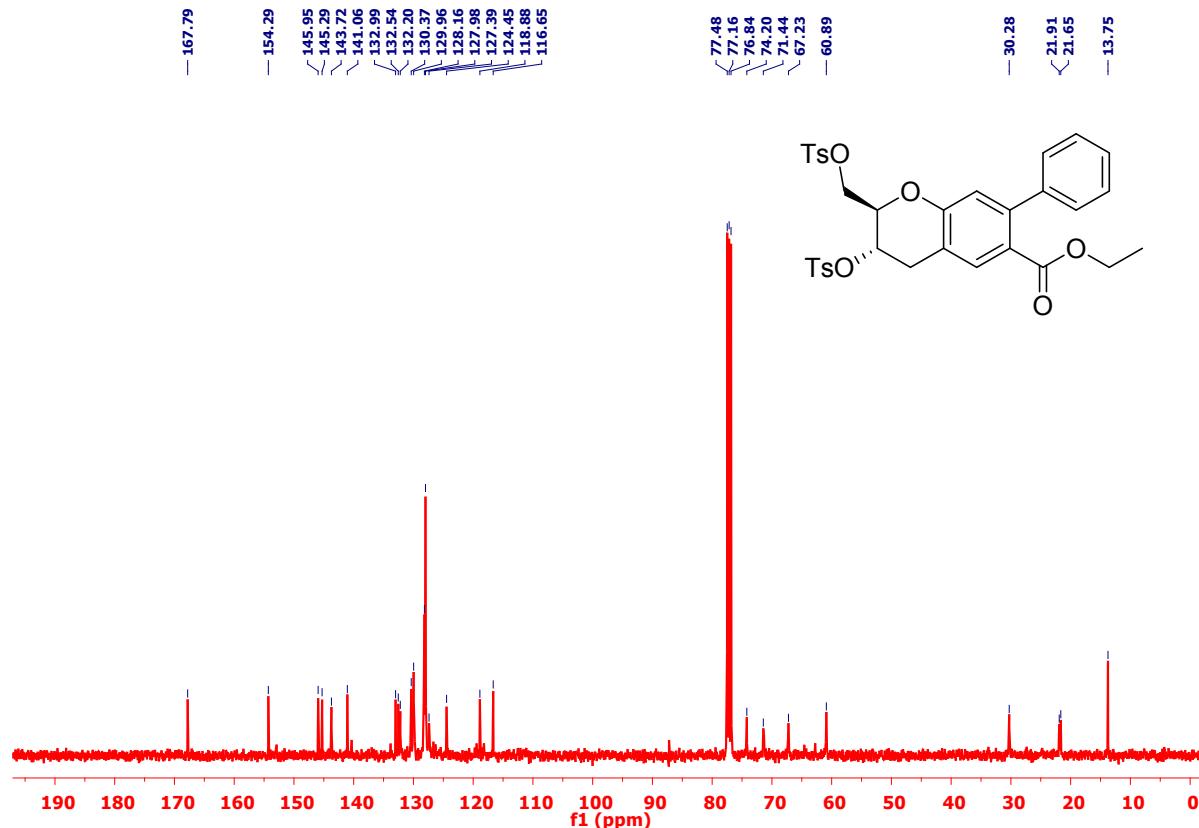


Figure S74. ¹³C NMR spectrum of compound 7 (100.6 MHz, CDCl₃)

References

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