

Supporting information

[1,5]-Hydride shift-cyclization *versus* C(sp²)-H Functionalization in the Knoevenagel-Cyclization Domino Reactions of 1,4- and 1,5-Benzoxazepines

Dóra Szalóki Vargáné ^{1,2,†}, László Tóth ^{1,3,†}, Balázs Buglyó ¹, Attila Kiss-Szikszai ¹, Attila Mándi ¹, Péter Mátyus ⁴, Sándor Antus ^{1,*}, Yinghan Chen ⁵, Dehai Li ⁵, Lingxue Tao ⁶, Haiyan Zhang ⁶ and Tibor Kurtán ^{1,*}

¹ Department of Organic Chemistry, University of Debrecen, Debrecen, P. O. Box 400, Debrecen 4002, Hungary; szalokido@gmail.com (D.S.V.); tothlaszlochemist@gmail.com (L.T.); buglyo.balazs@science.unideb.hu (B.B.); kiss.attila@science.unideb.hu (A.K.-S.); mandi.attila@science.unideb.hu (A.M.)

² Doctoral School of Chemistry, University of Debrecen, Egyetem tér 1, Debrecen 4032, Hungary

³ Department of Organic Chemistry, Semmelweis University, Budapest 1094, Hungary

⁴ Institute of Digital Health Sciences, Faculty of Health and Public Services, Semmelweis University, Ferenc tér 15, Budapest 1094, Hungary; peter.maty@gmail.com

⁵ Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, China; qd_yinghan@163.com (Y.C.); dehaili@ouc.edu.cn (D.L.);

⁶ CAS Key Laboratory of Receptor Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zu Chong Zhi Road, Zhang Jiang Hi-Tech Park, Shanghai 201203, China; lingxuetao@simm.ac.cn (L.T.); hzhang@simm.ac.cn (H.Z.)

* Correspondences: kurtan.tibor@science.unideb.hu (T.K.), antus.sandor@science.unideb.hu (S.A.)

† These authors contributed equally to this work.

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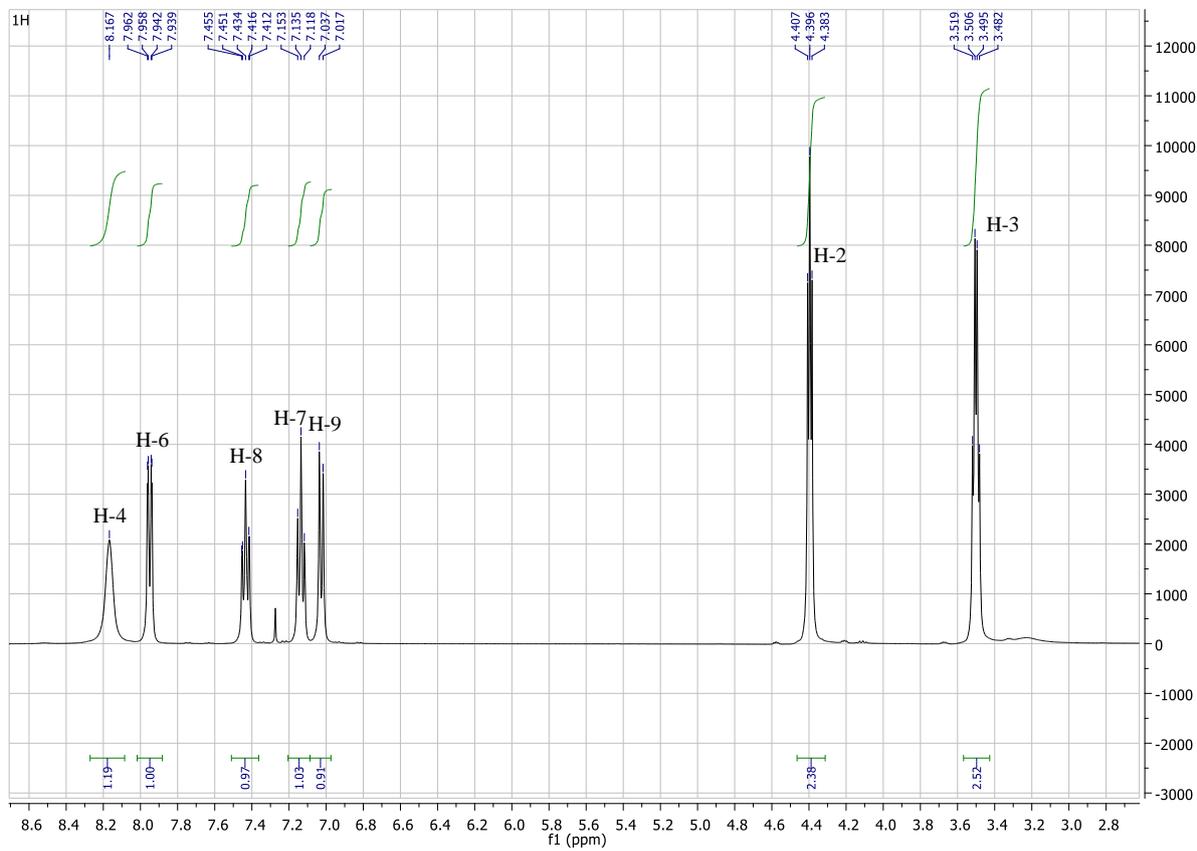
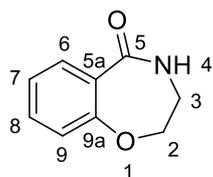


Figure S1. ¹H-NMR spectrum of *rac*-8a measured in CDCl₃ (400 MHz).

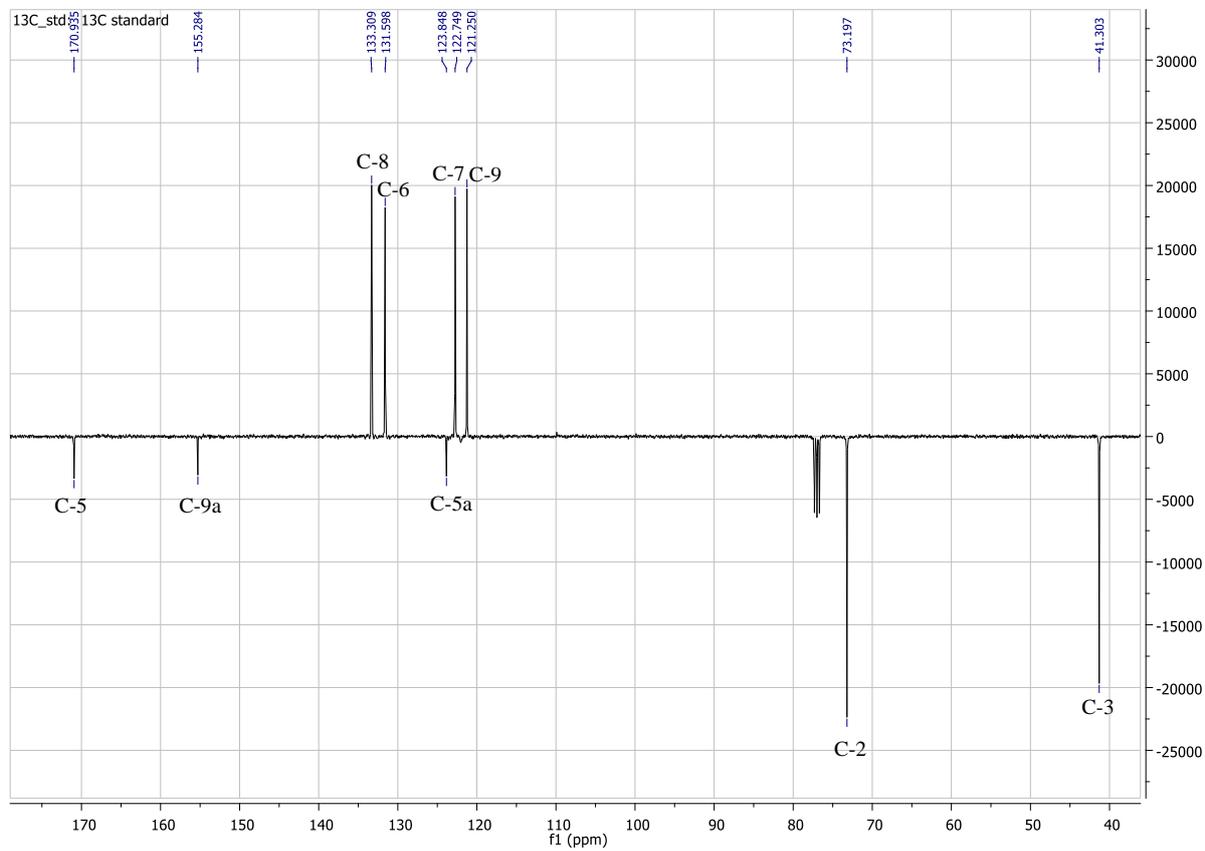
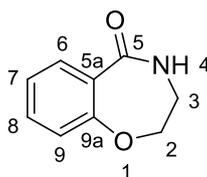


Figure S2. J-modulated ¹³C-NMR spectrum of *rac*-**8a** measured in CDCl₃ (100 MHz).

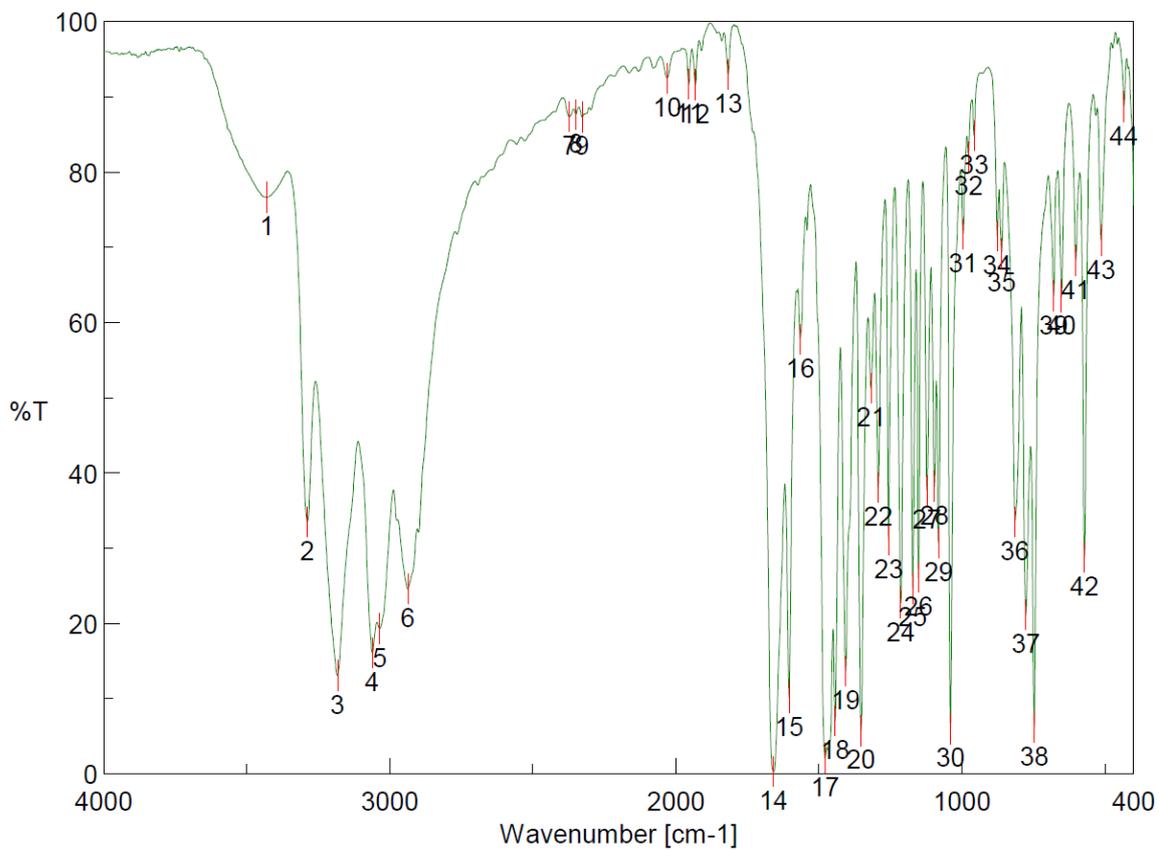
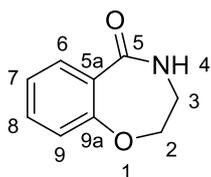


Figure S3. IR spectrum of *rac*-8a recorded as KBr disc.

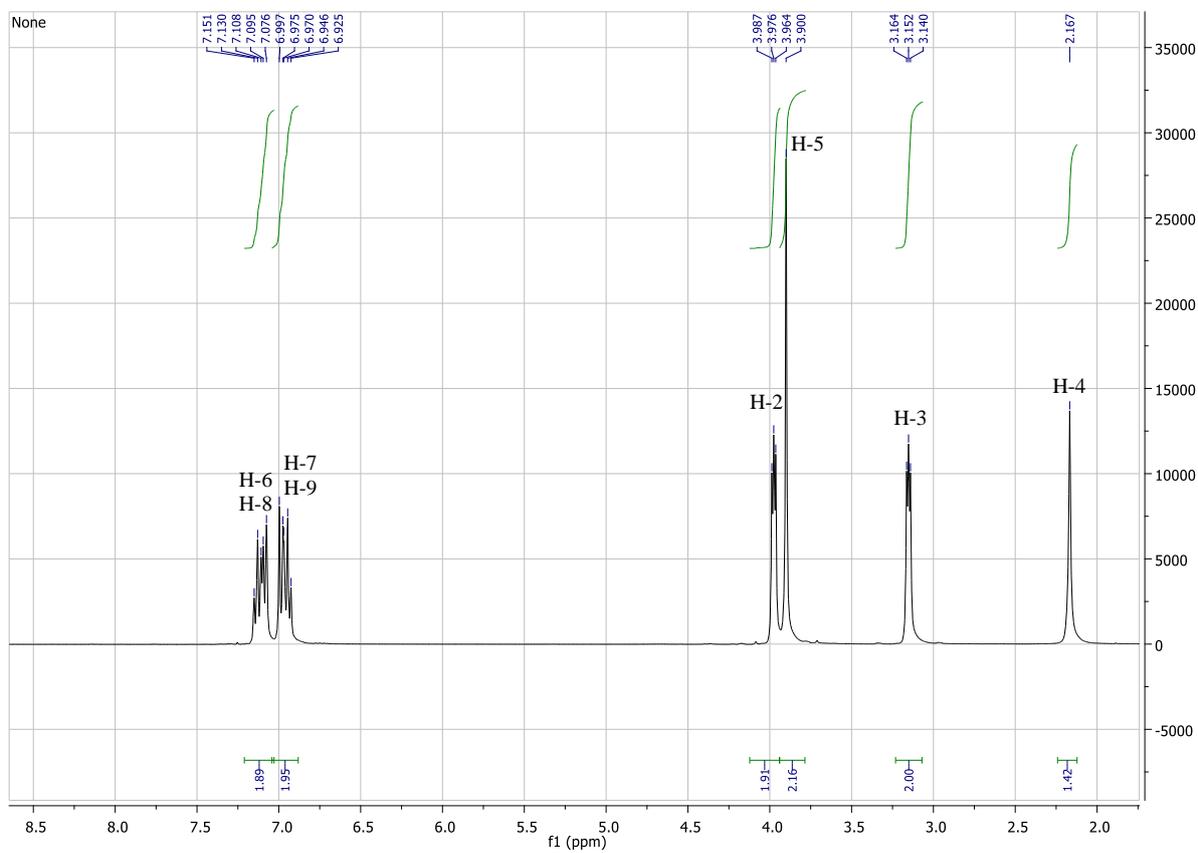
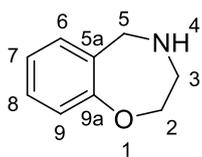


Figure S4. $^1\text{H-NMR}$ spectrum of *rac-9a* measured in CDCl_3 (400 MHz).

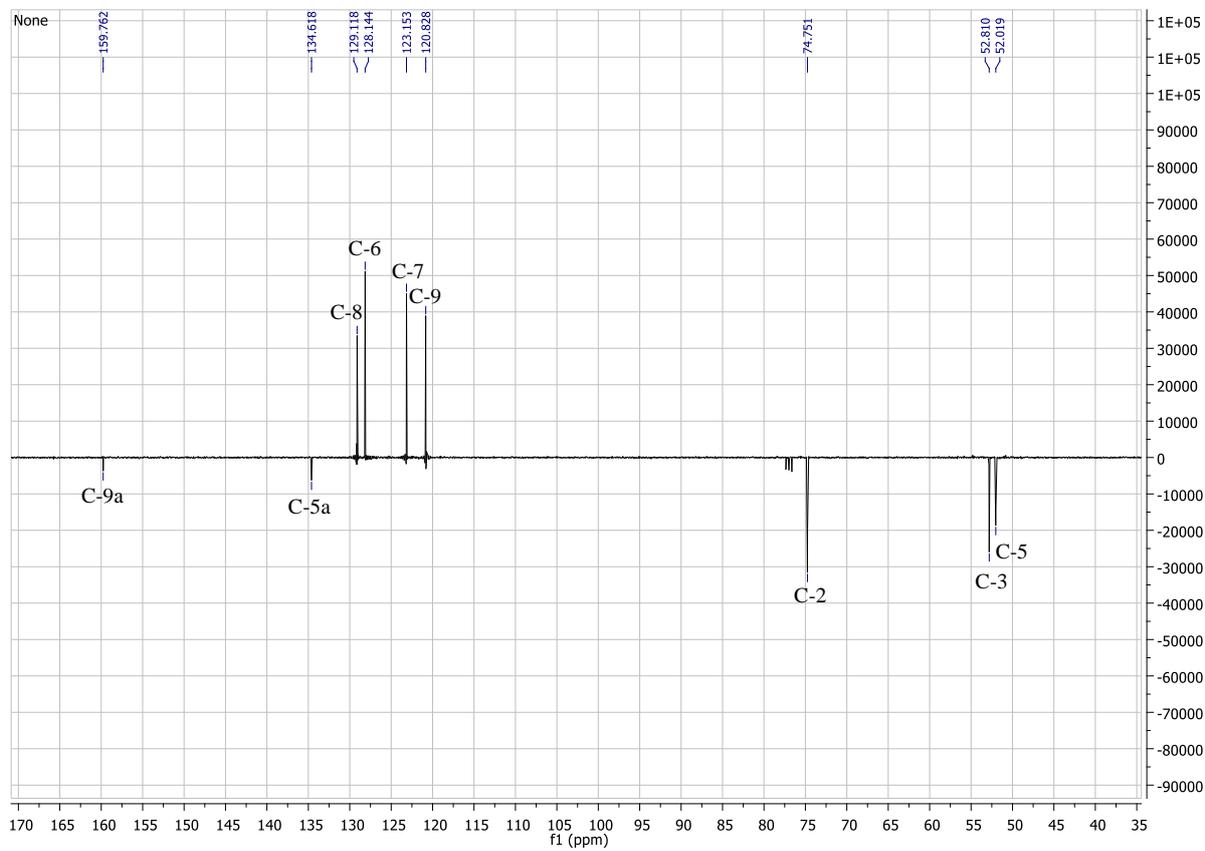
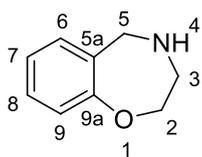


Figure S5. J-modulated ¹³C-NMR spectrum of *rac-9a* measured in CDCl₃ (100 MHz).

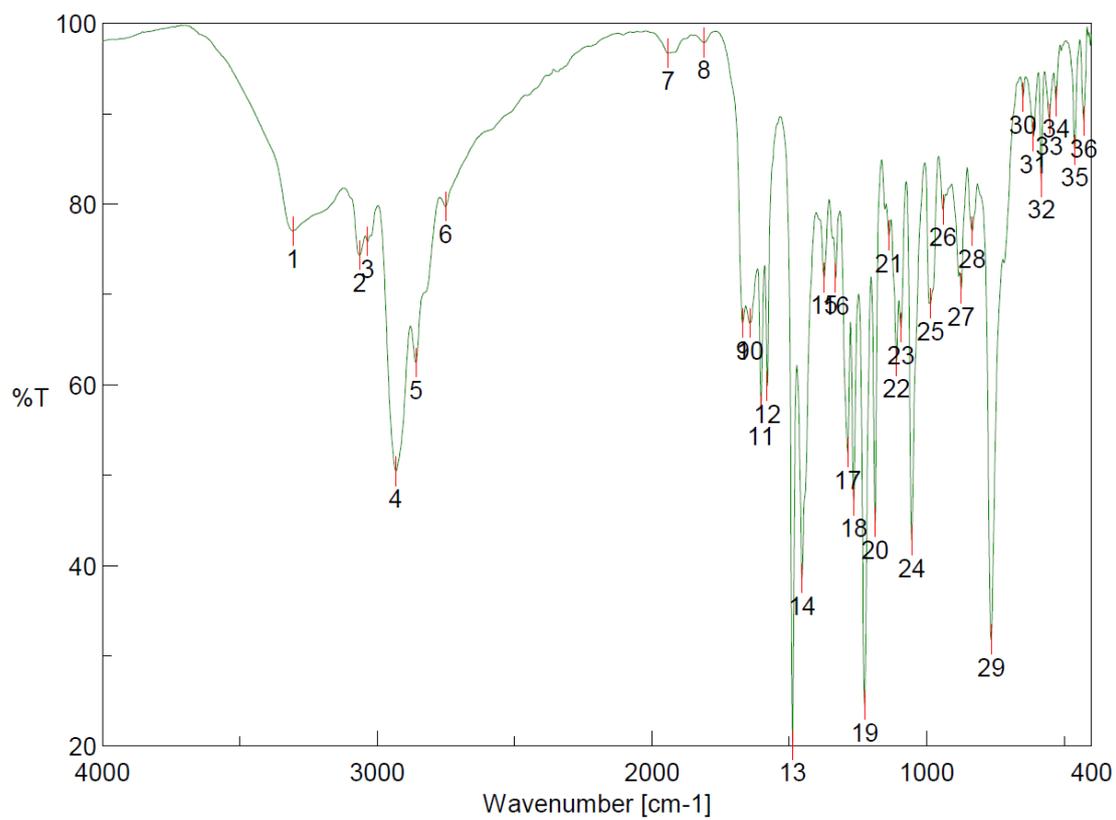
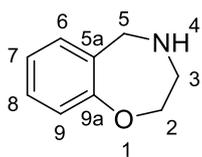


Figure S6. IR spectrum of *rac*-9a recorded as KBr disc.

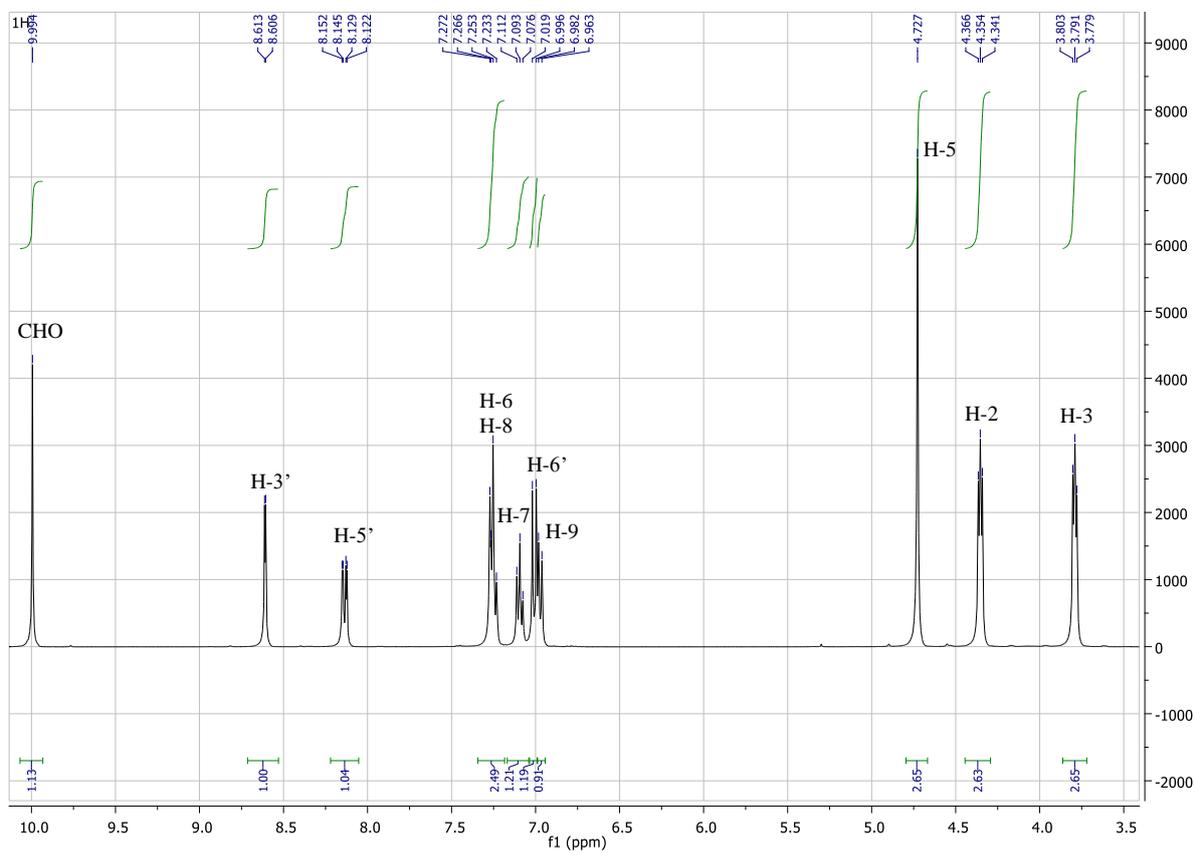
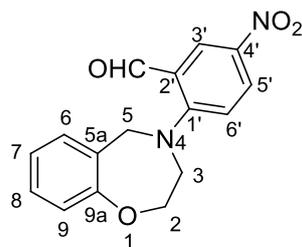


Figure S7. $^1\text{H-NMR}$ spectrum of *rac-1a* measured in CDCl_3 (400 MHz).

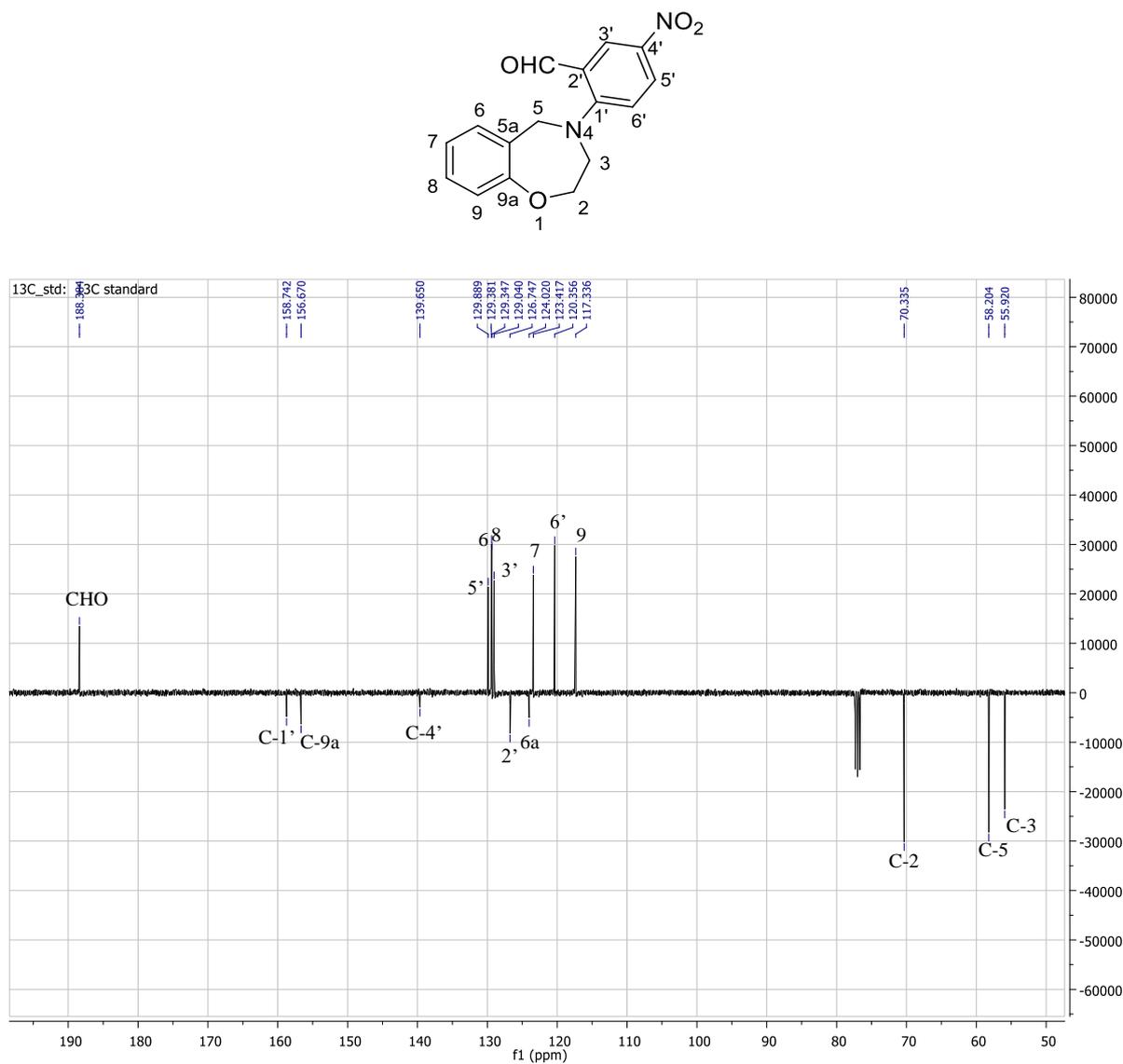


Figure S8. J-modulated ¹³C-NMR spectrum of *rac-1a* measured in CDCl₃ (100 MHz).

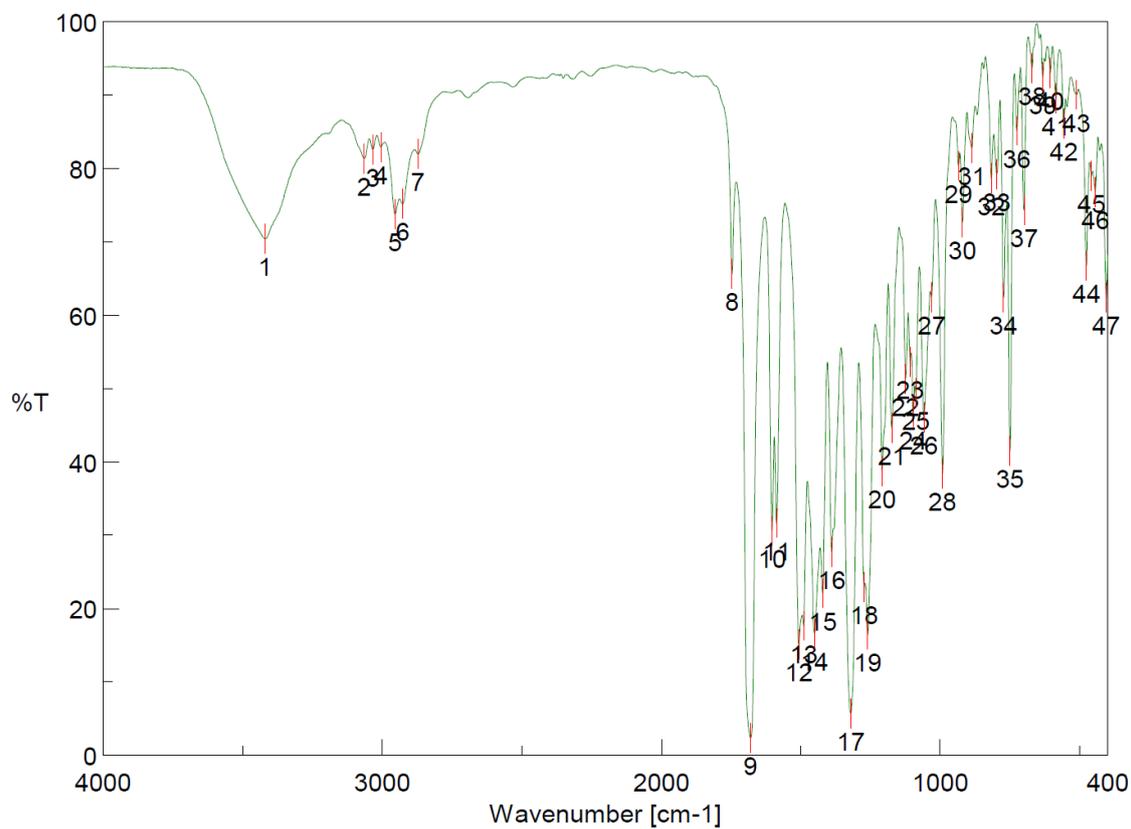
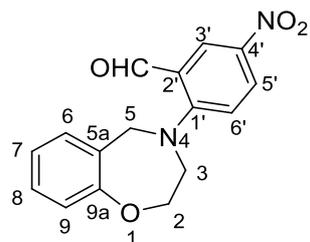


Figure S9. IR spectrum of *rac-1a* recorded as KBr disc.

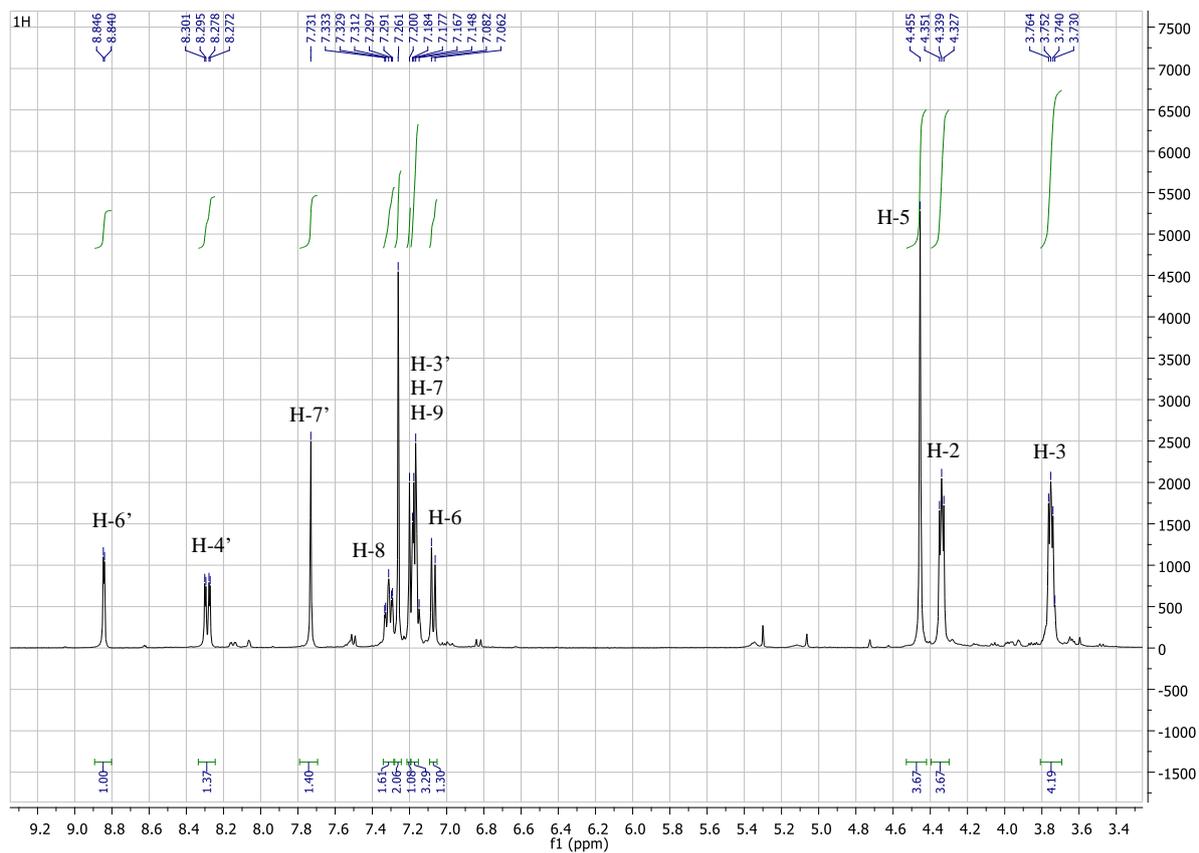
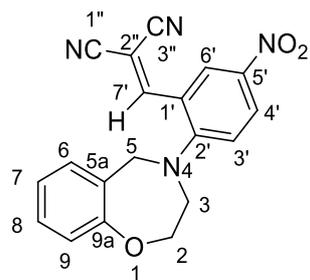


Figure S10. $^1\text{H-NMR}$ spectrum of *rac-12a* measured in CDCl_3 (400 MHz).

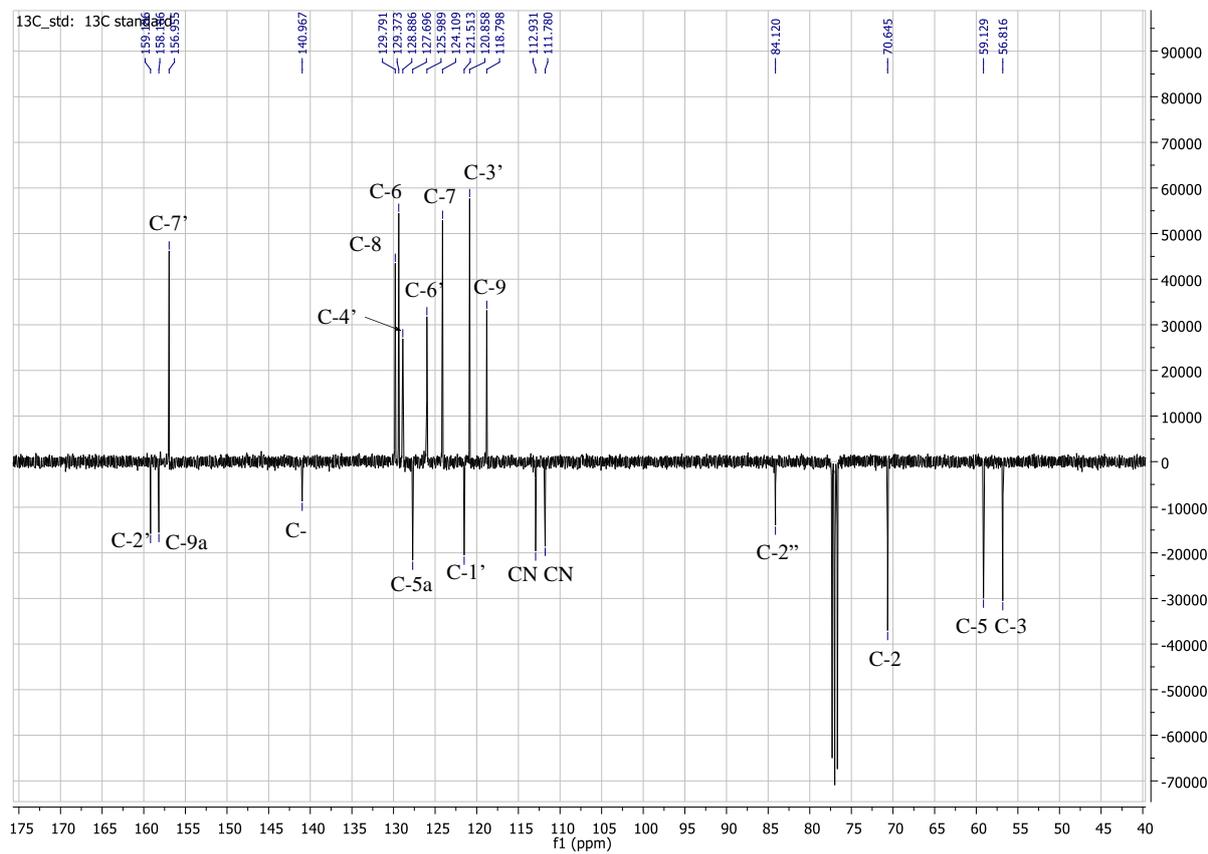
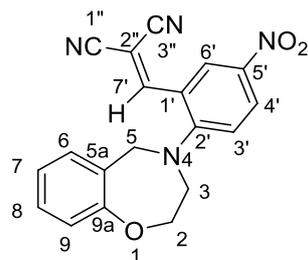


Figure S11. J-modulated ¹³C-NMR spectrum of *rac-12a* measured in CDCl₃ (100 MHz).

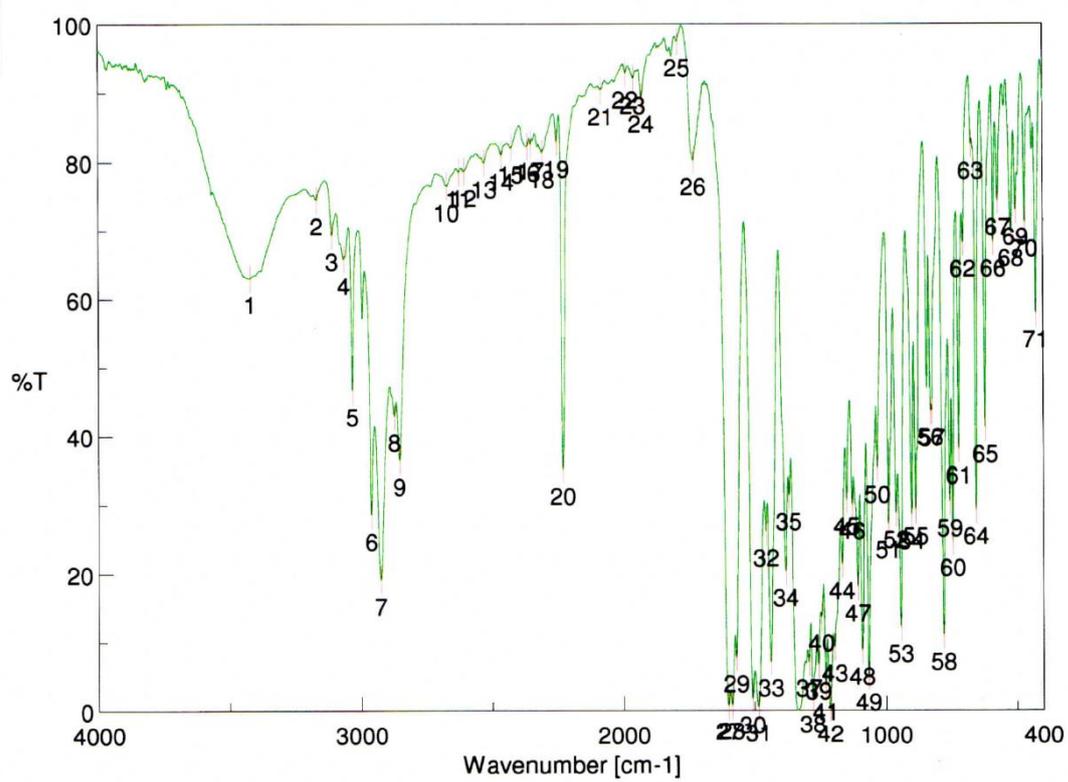
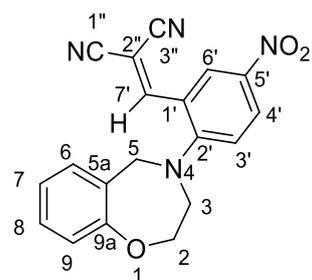


Figure S12. IR spectrum of *rac*-**12a** recorded as KBr disc.

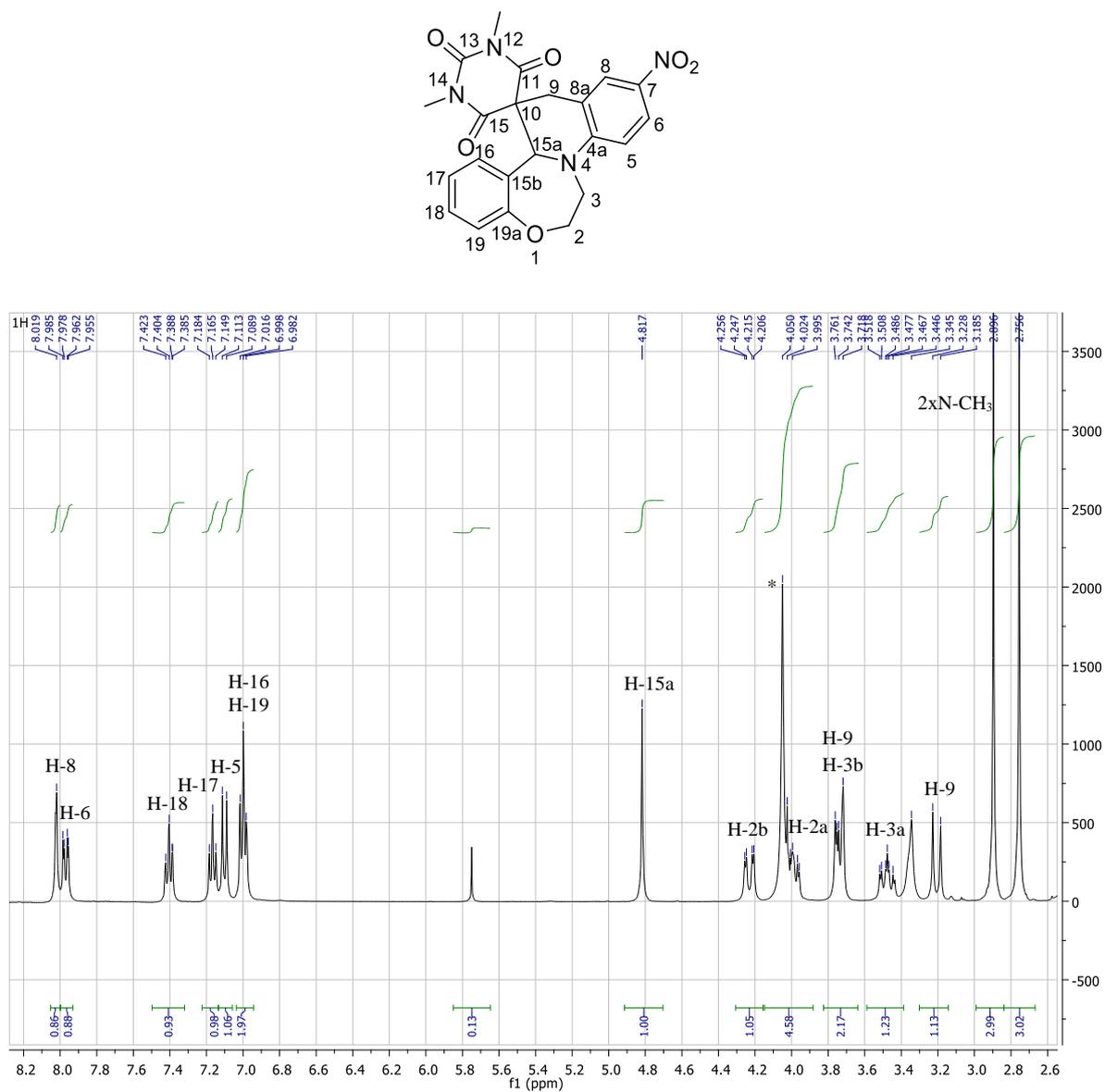


Figure S13. ¹H-NMR spectrum of *rac*-10a measured in CDCl₃ (400 MHz).

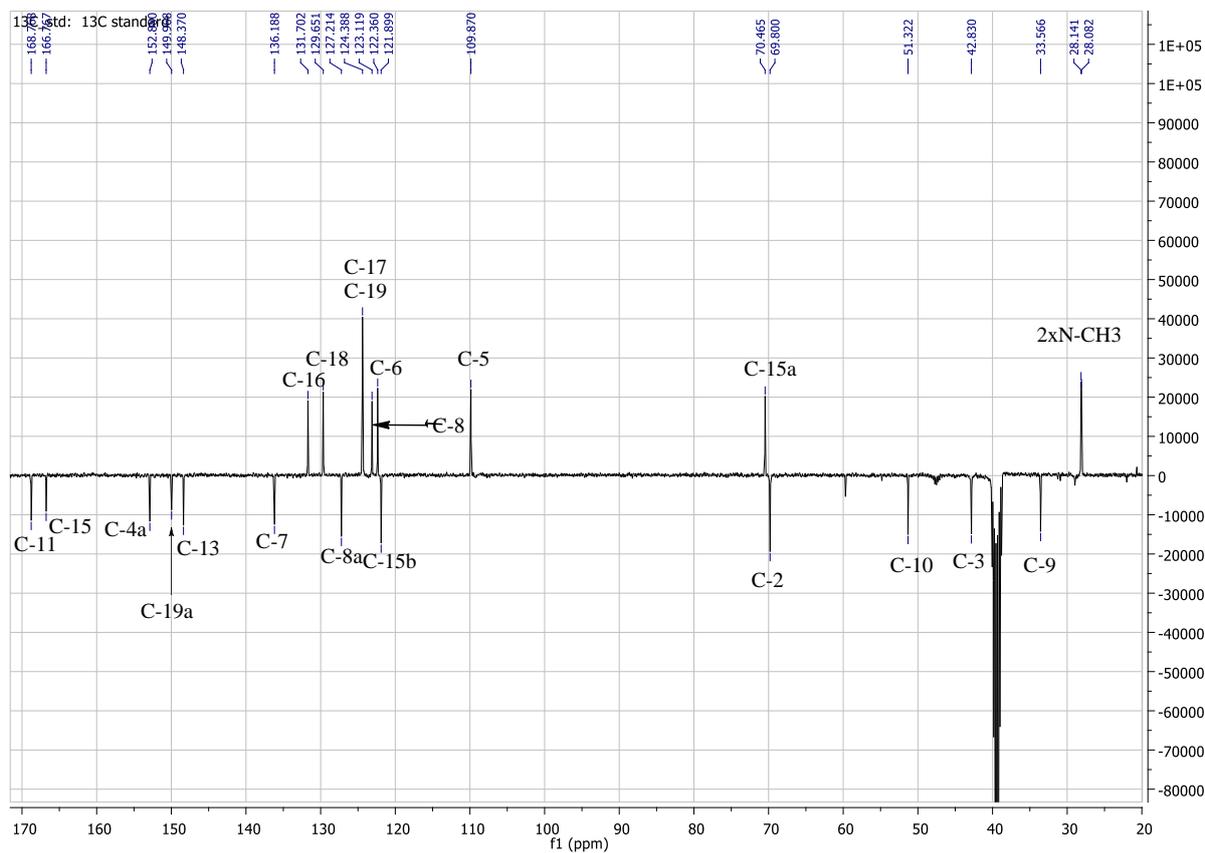
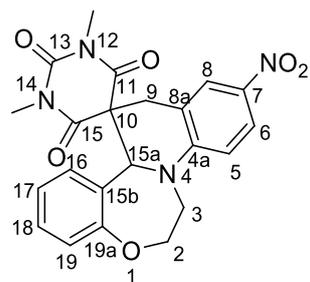


Figure S14. J-modulated ^{13}C -NMR spectrum of *rac*-**10a** measured in CDCl_3 (100 MHz).

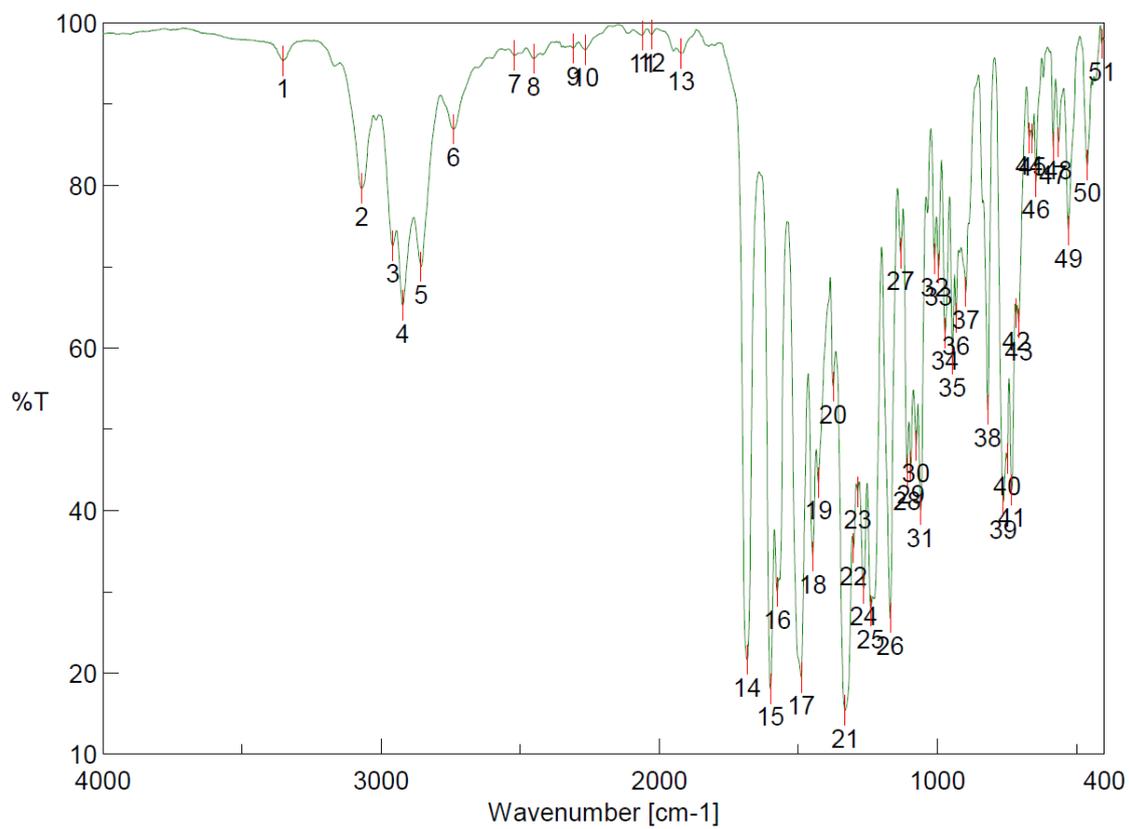
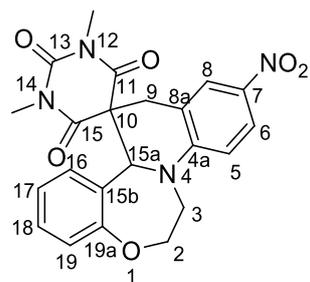


Figure S15. IR spectrum of *rac*-10a recorded as KBr disc

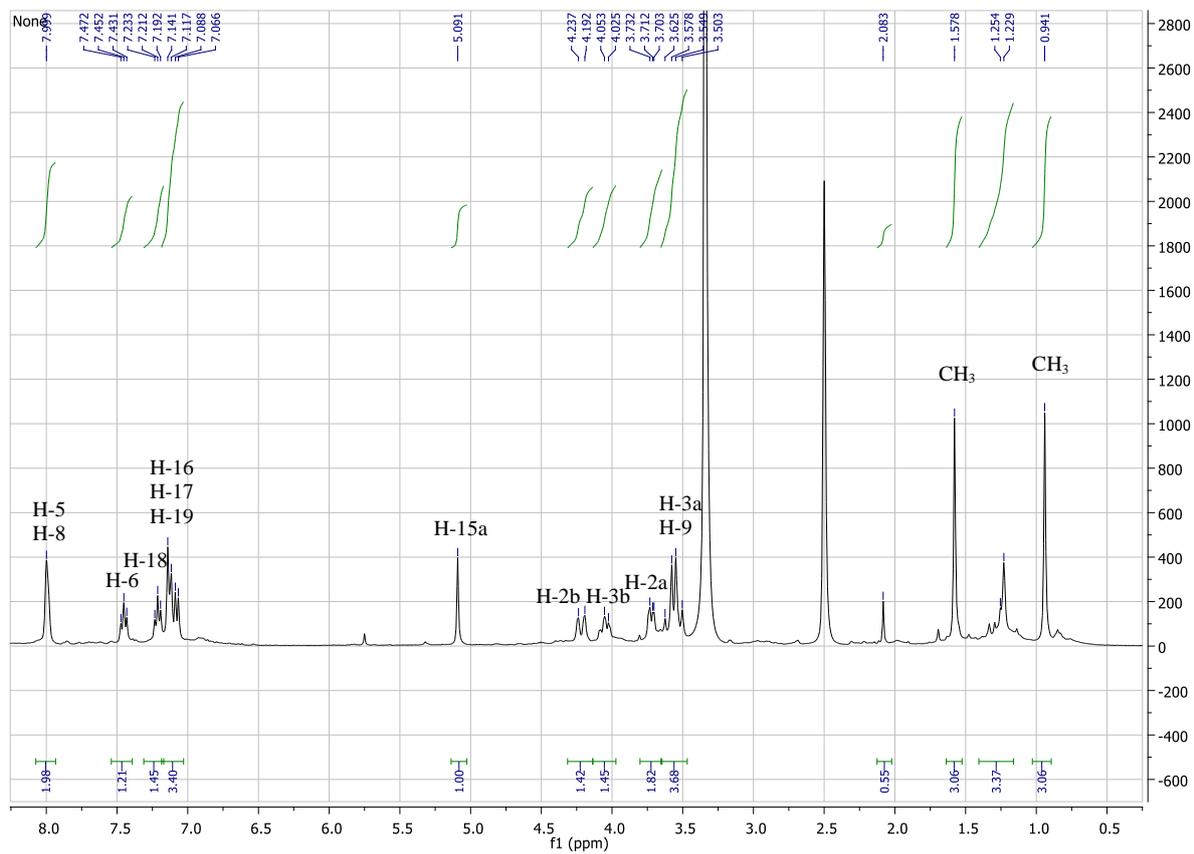
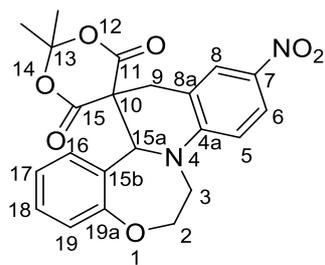


Figure S16. ¹H-NMR spectrum of *rac*-11a measured in DMSO-d₆ (400 MHz)

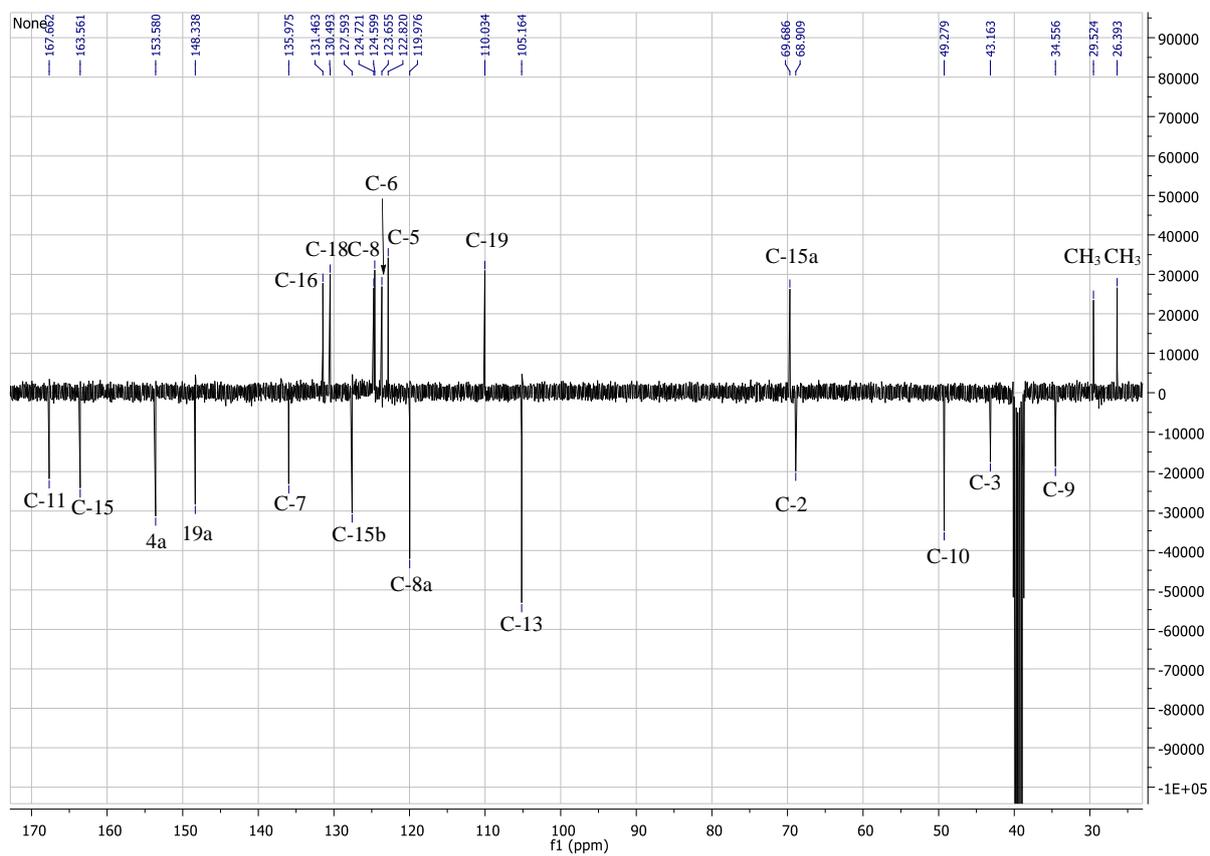
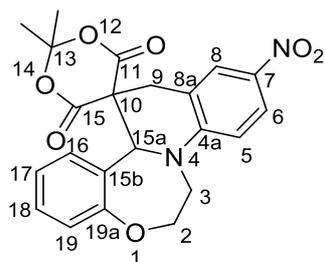


Figure S17. J-modulated ¹³C-NMR spectrum of *rac*-**11a** measured in DMSO-d₆ (100 MHz)

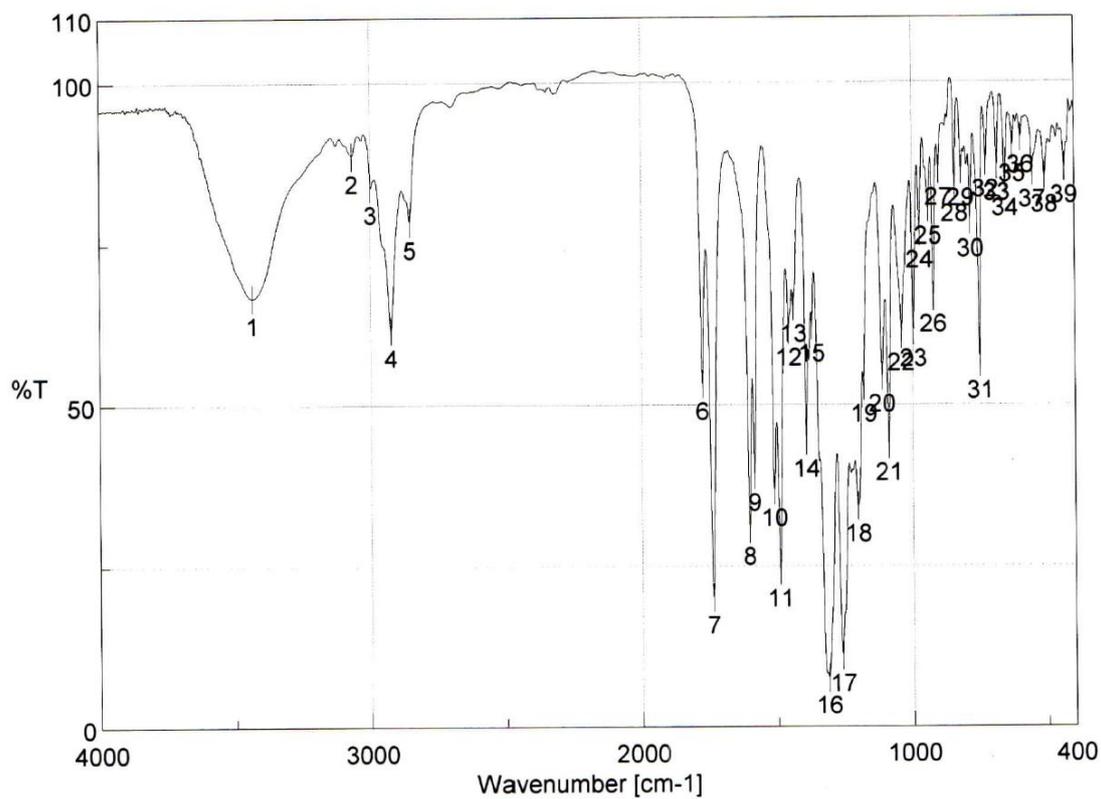
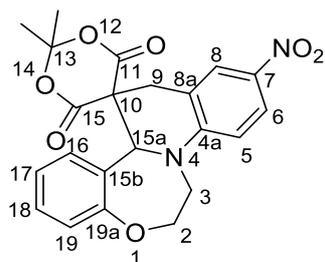


Figure S18. IR spectrum of *rac*-11a recorded as KBr disc

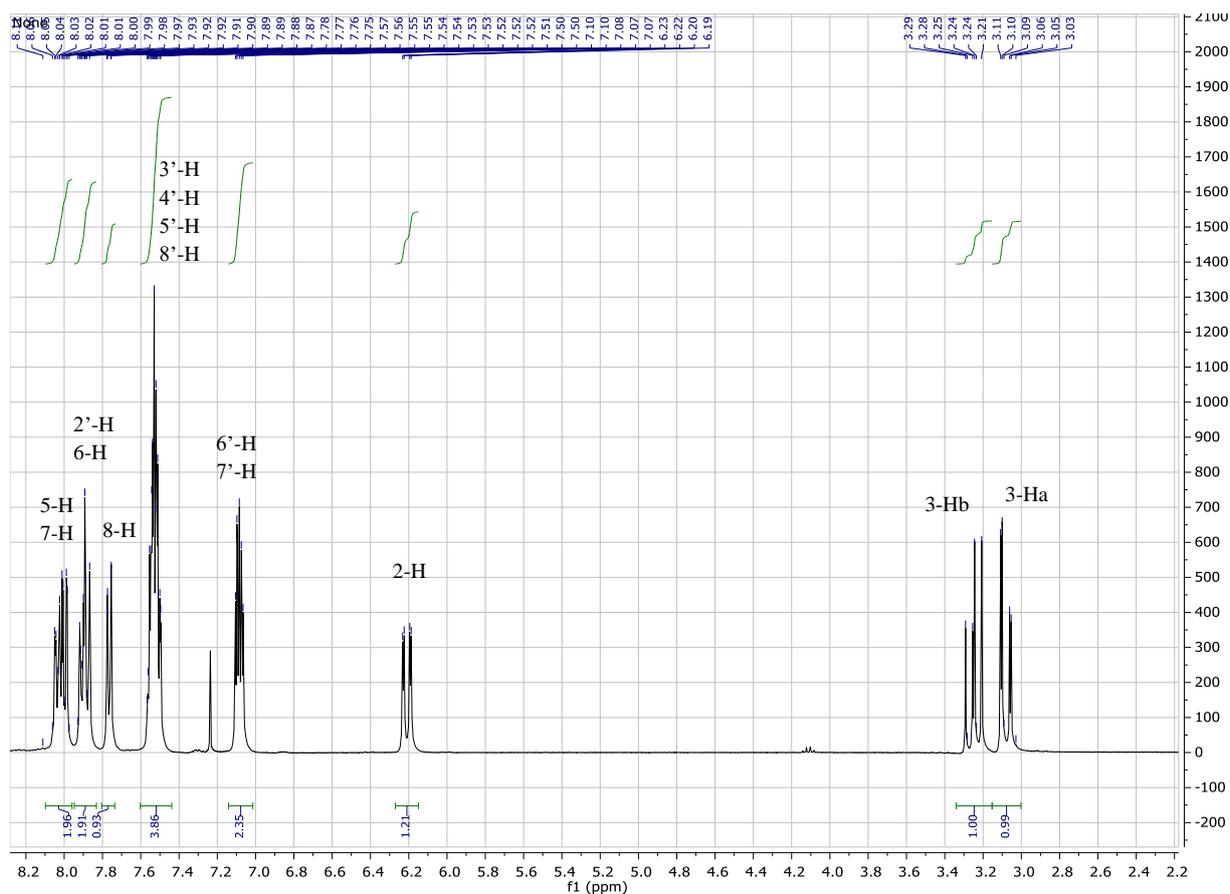
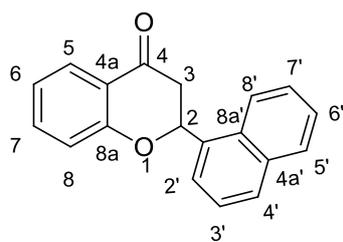


Figure S19. $^1\text{H-NMR}$ spectrum of *rac-7b* measured in CDCl_3 (360 MHz)

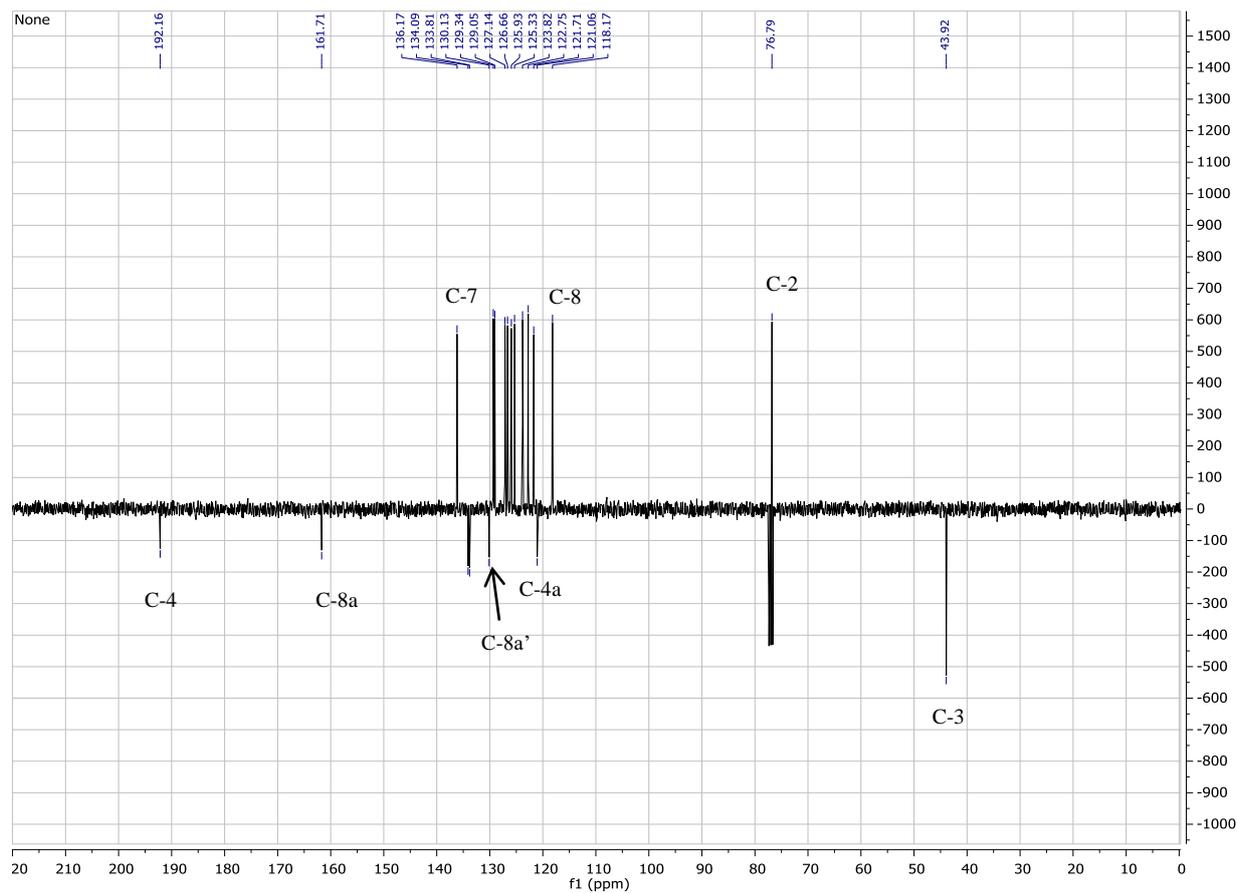
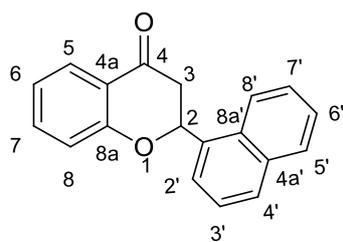


Figure S20. J-modulated ^{13}C -NMR spectrum of *rac-7b* measured in CDCl_3 (90 MHz)

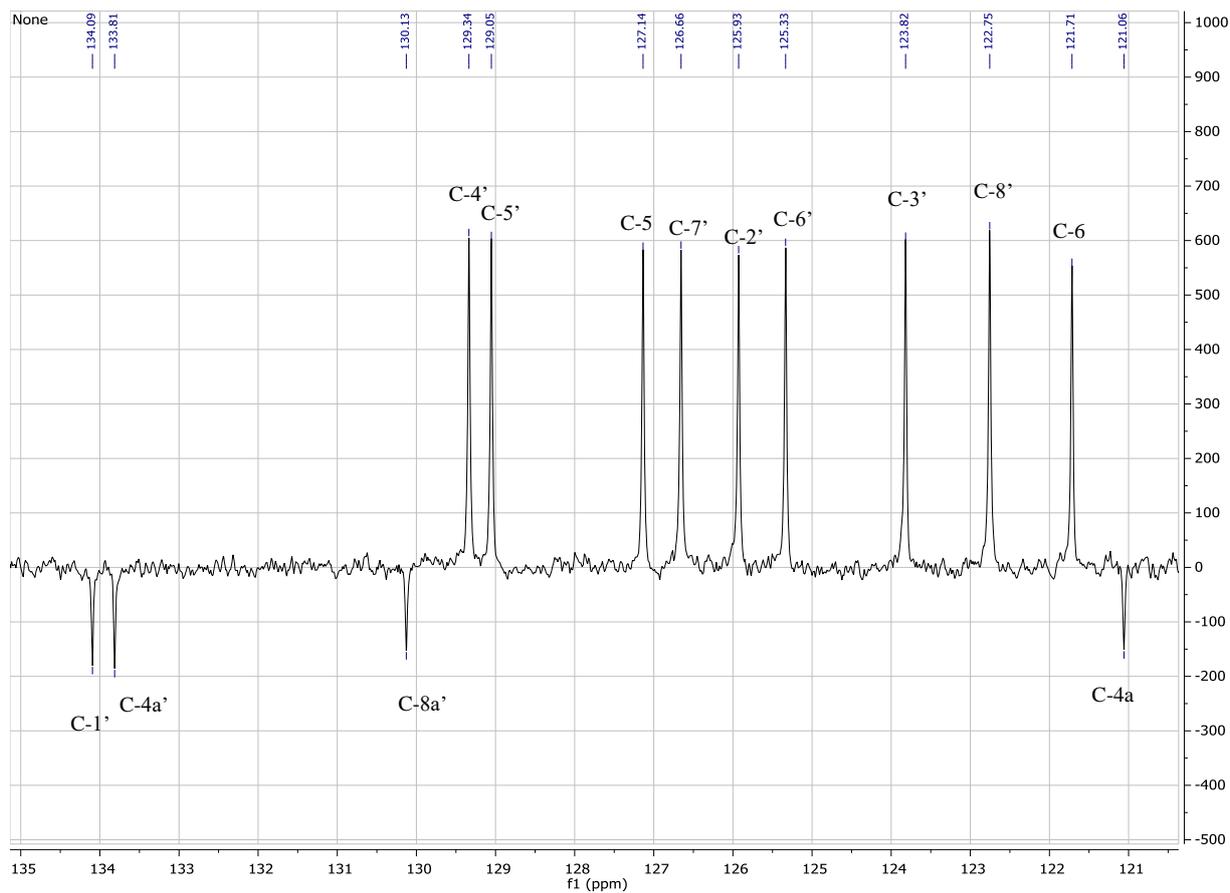
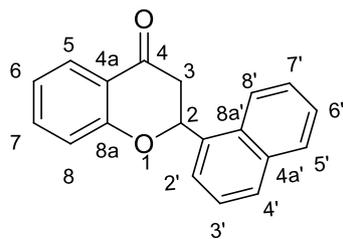


Figure S21. J-modulated ^{13}C -NMR spectrum of *rac*-**7b** measured in CDCl_3 (90 MHz)

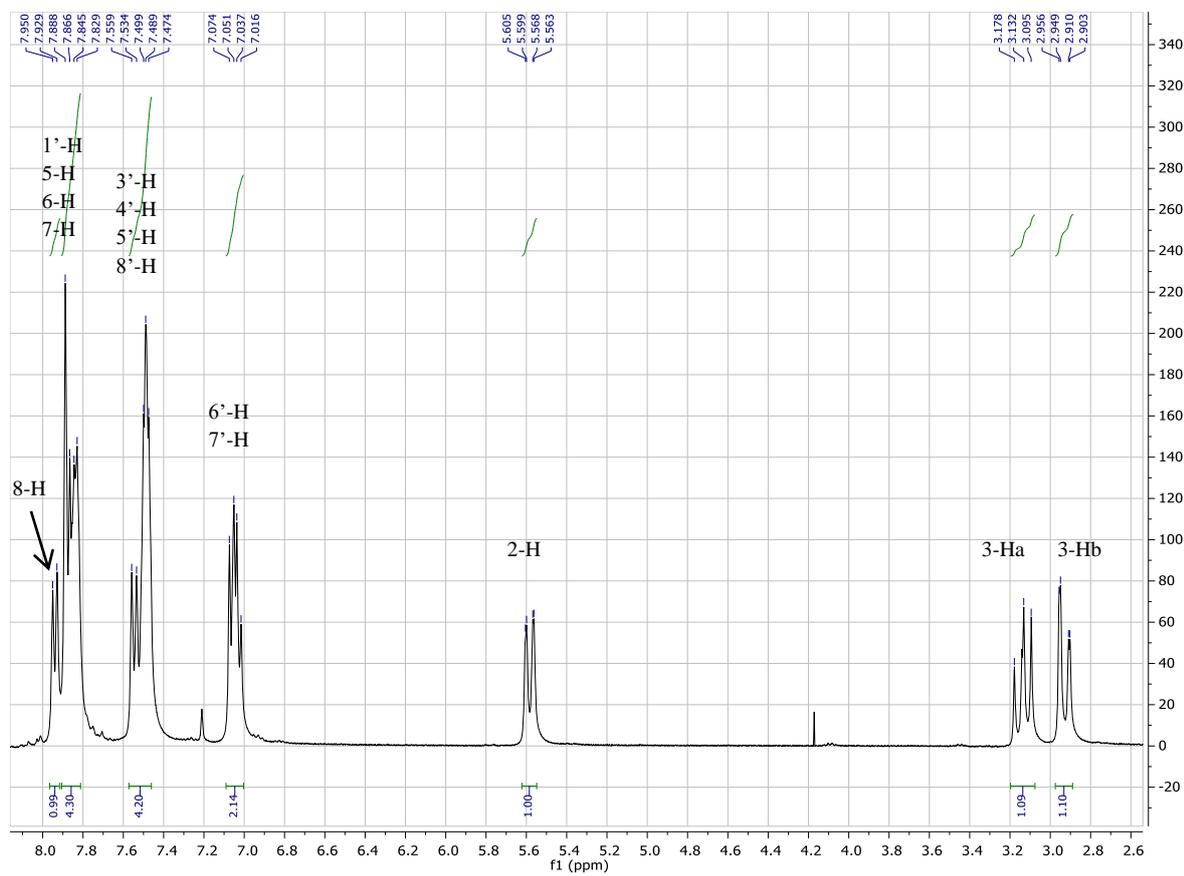
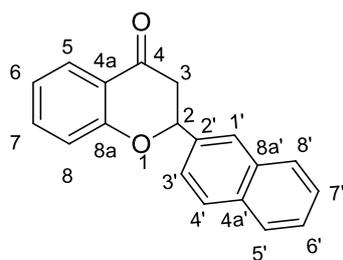


Figure S22. ¹H-NMR spectrum of *rac-7c* measured in CDCl₃ (360 MHz)

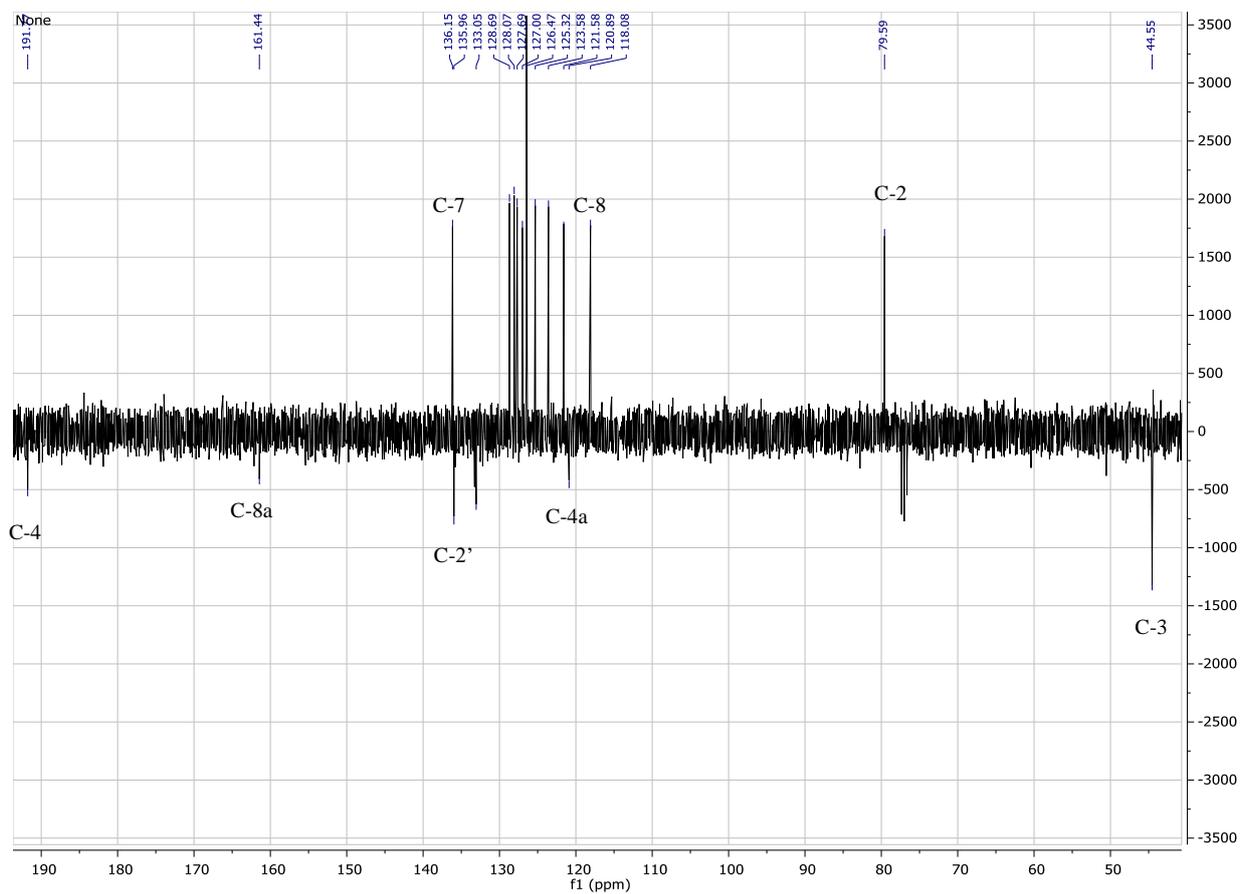
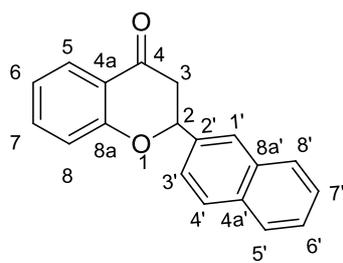


Figure S23. J-modulated ^{13}C -NMR spectrum of *rac-7c* measured in CDCl_3 (90 MHz)

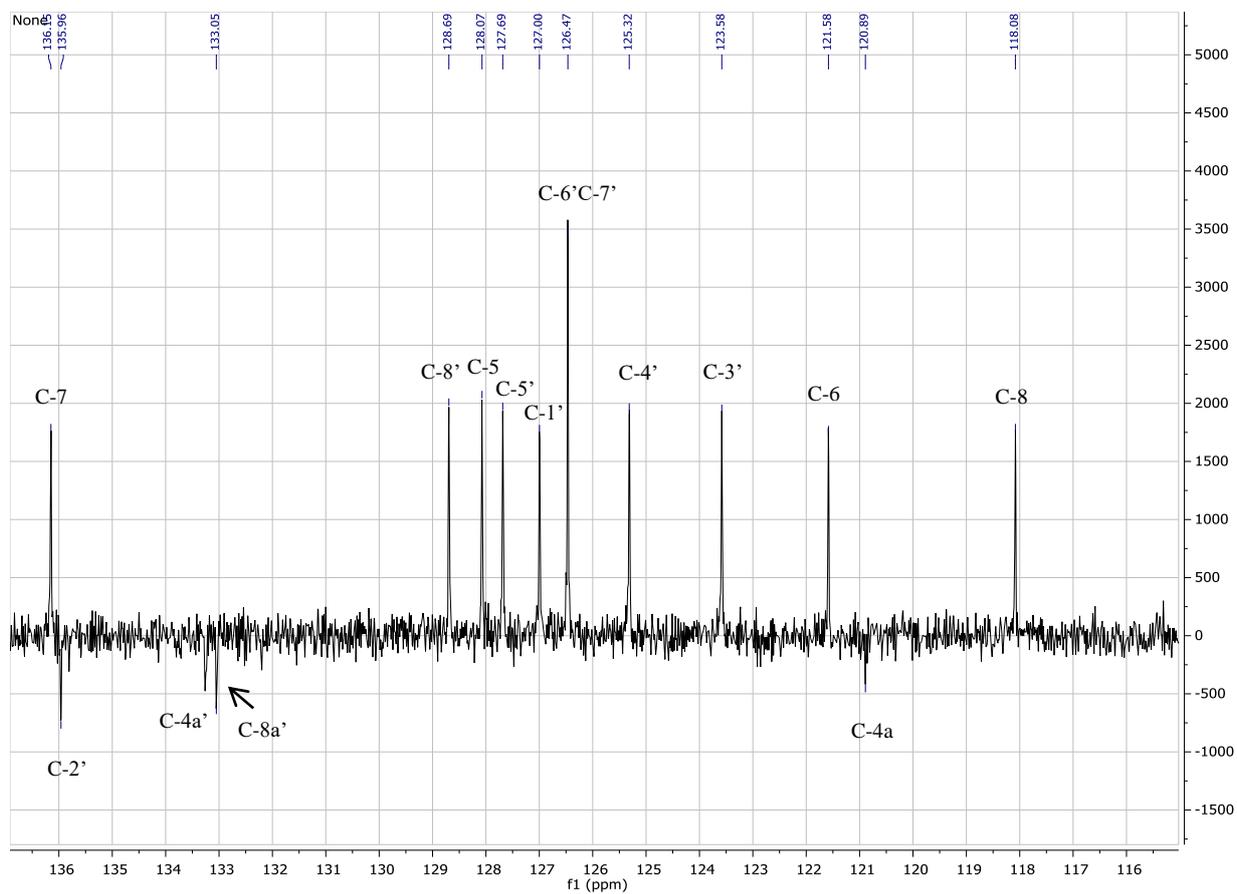
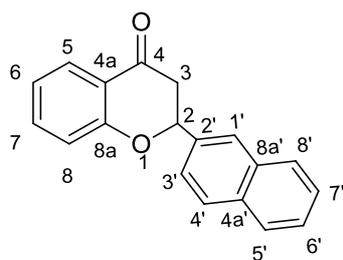


Figure S24. J-modulated ^{13}C -NMR spectrum of *rac*-7c measured in CDCl_3 (90 MHz)

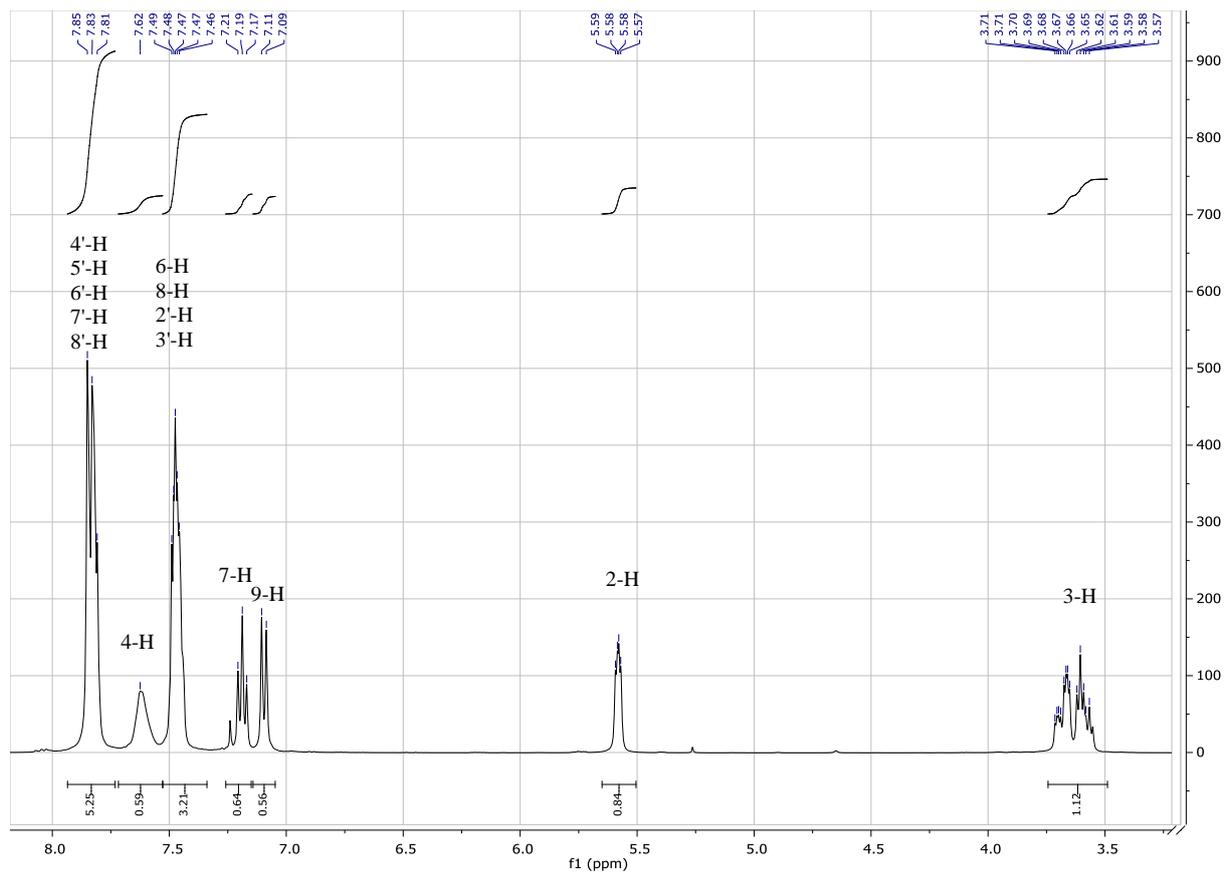
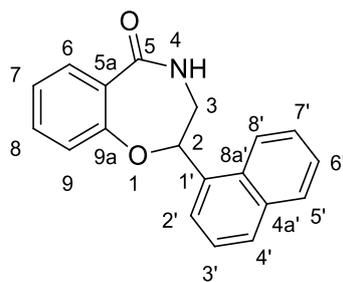


Figure S25. $^1\text{H-NMR}$ spectrum of *rac*-**8b** measured in CDCl_3 (400 MHz)

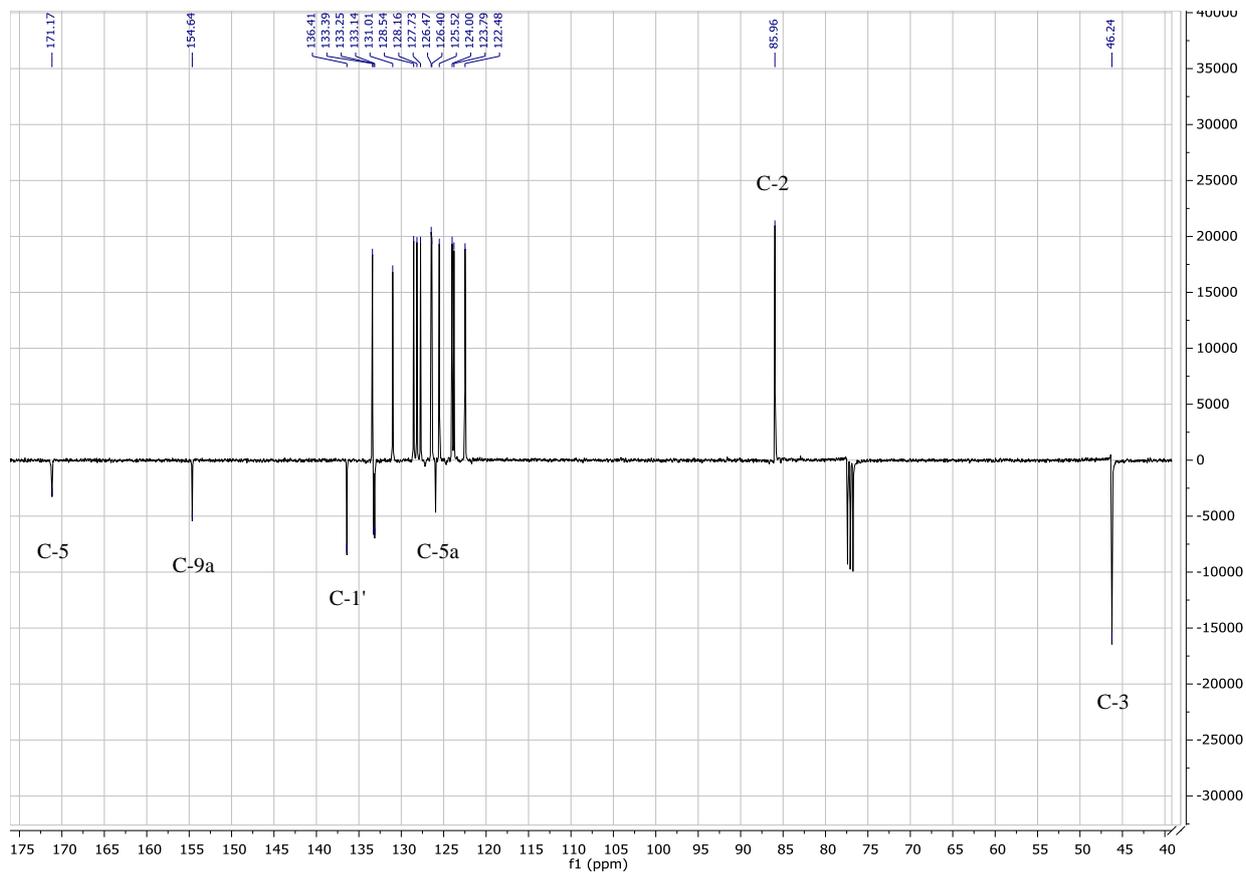
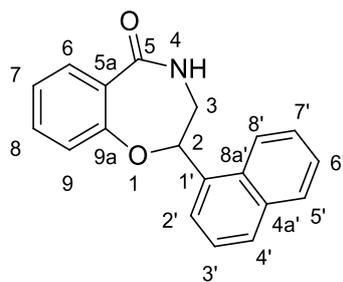


Figure S26. J-modulated ^{13}C -NMR spectrum of *rac*-**8b** measured in CDCl_3 (100 MHz)

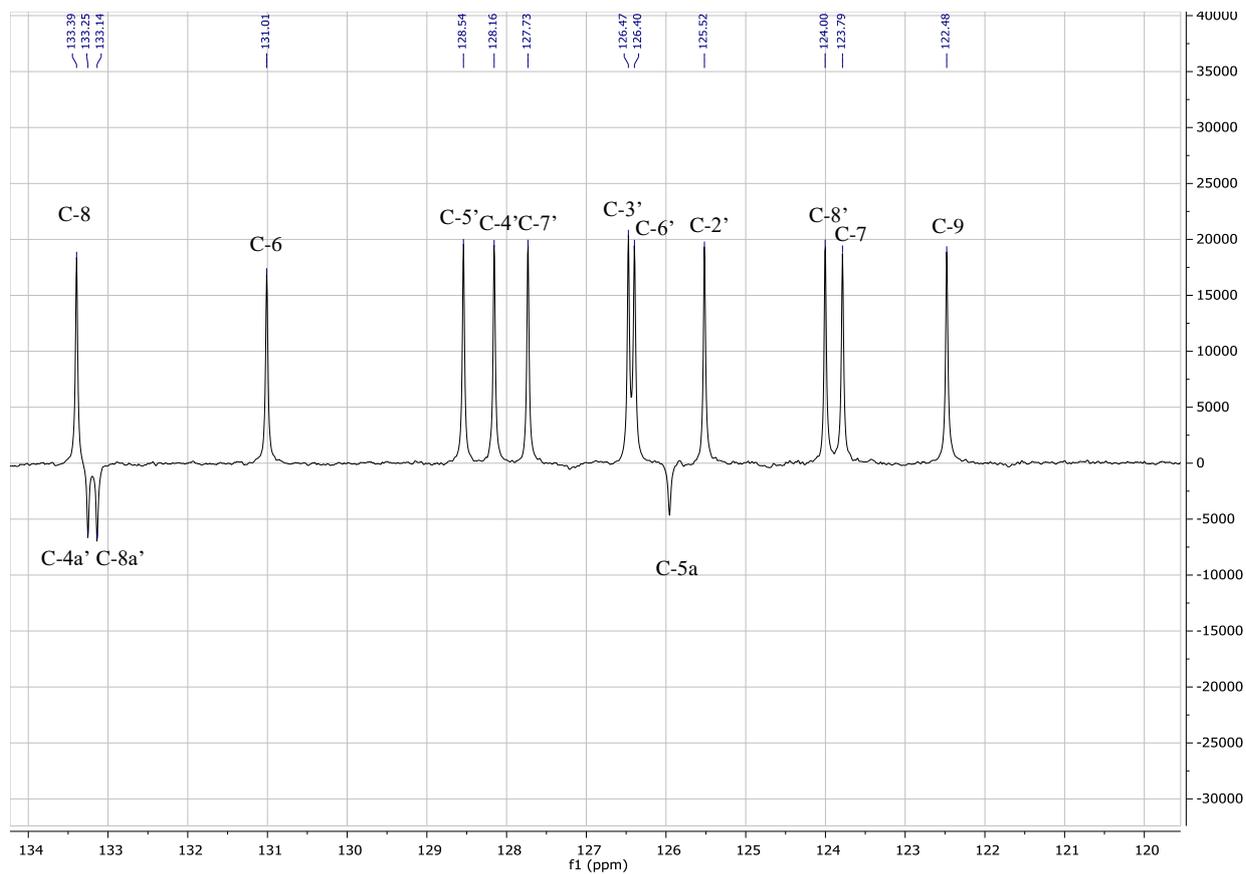
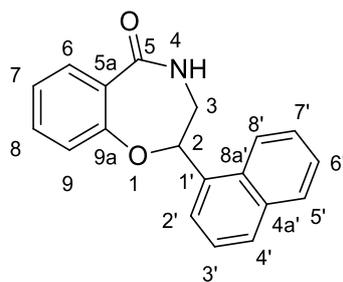


Figure S27. J-modulated ^{13}C -NMR spectra of *rac*-**8b** measured in CDCl_3 (100 MHz)

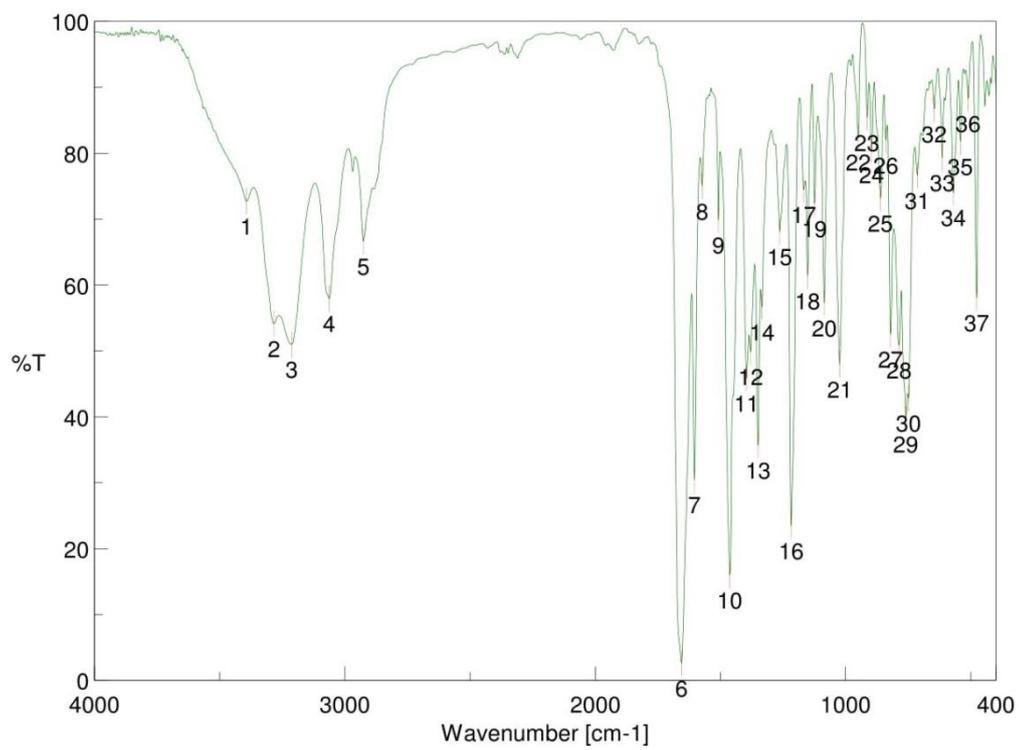
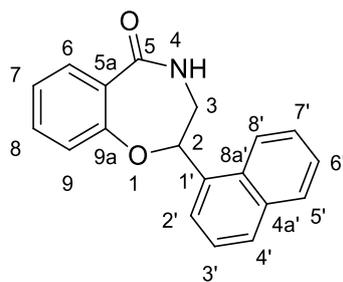


Figure S28 IR spectra of *rac-8b* recorded as KBr disc

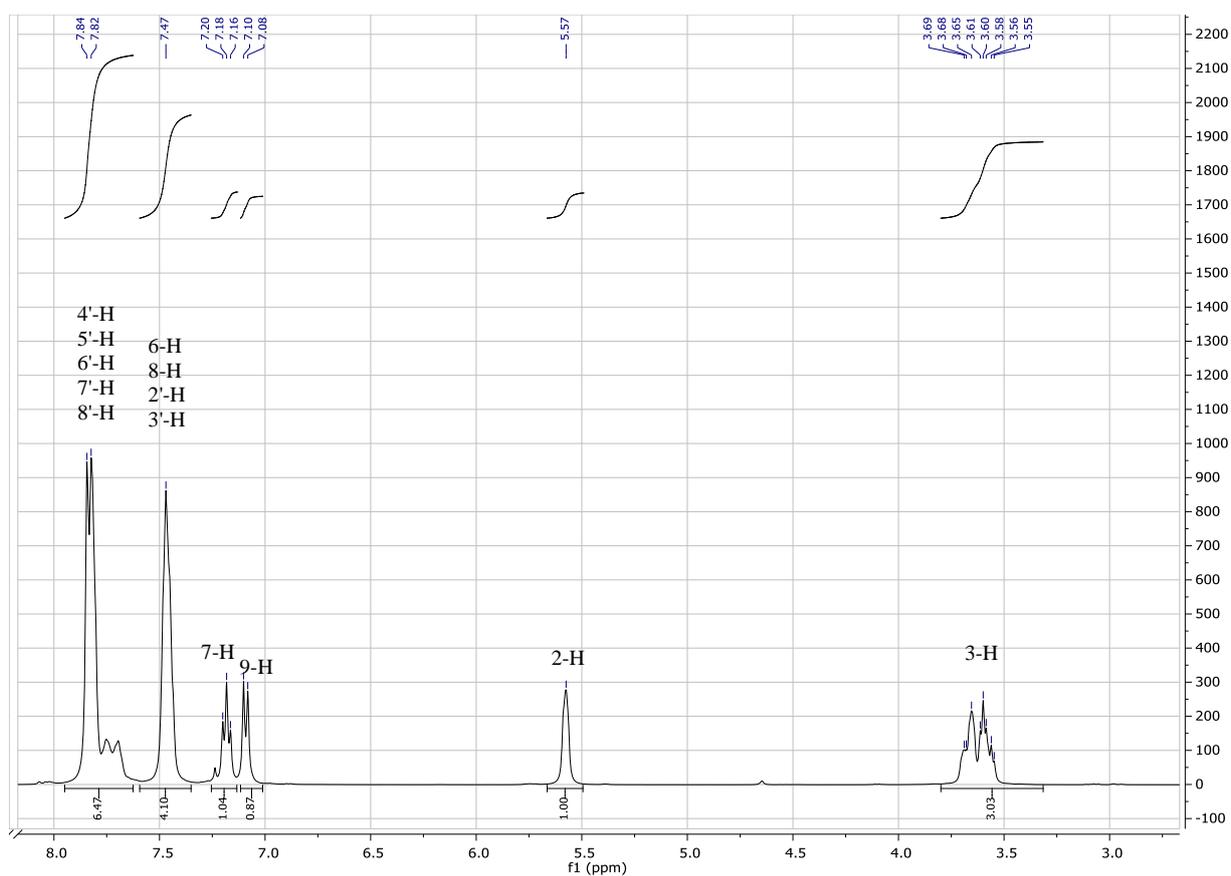
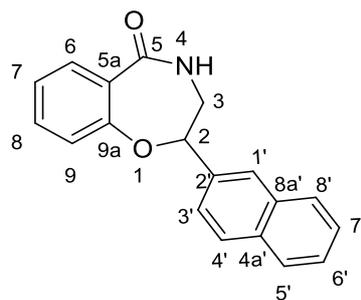


Figure S29. $^1\text{H-NMR}$ spectrum of *rac-8c* measured in CDCl_3 (400 MHz)

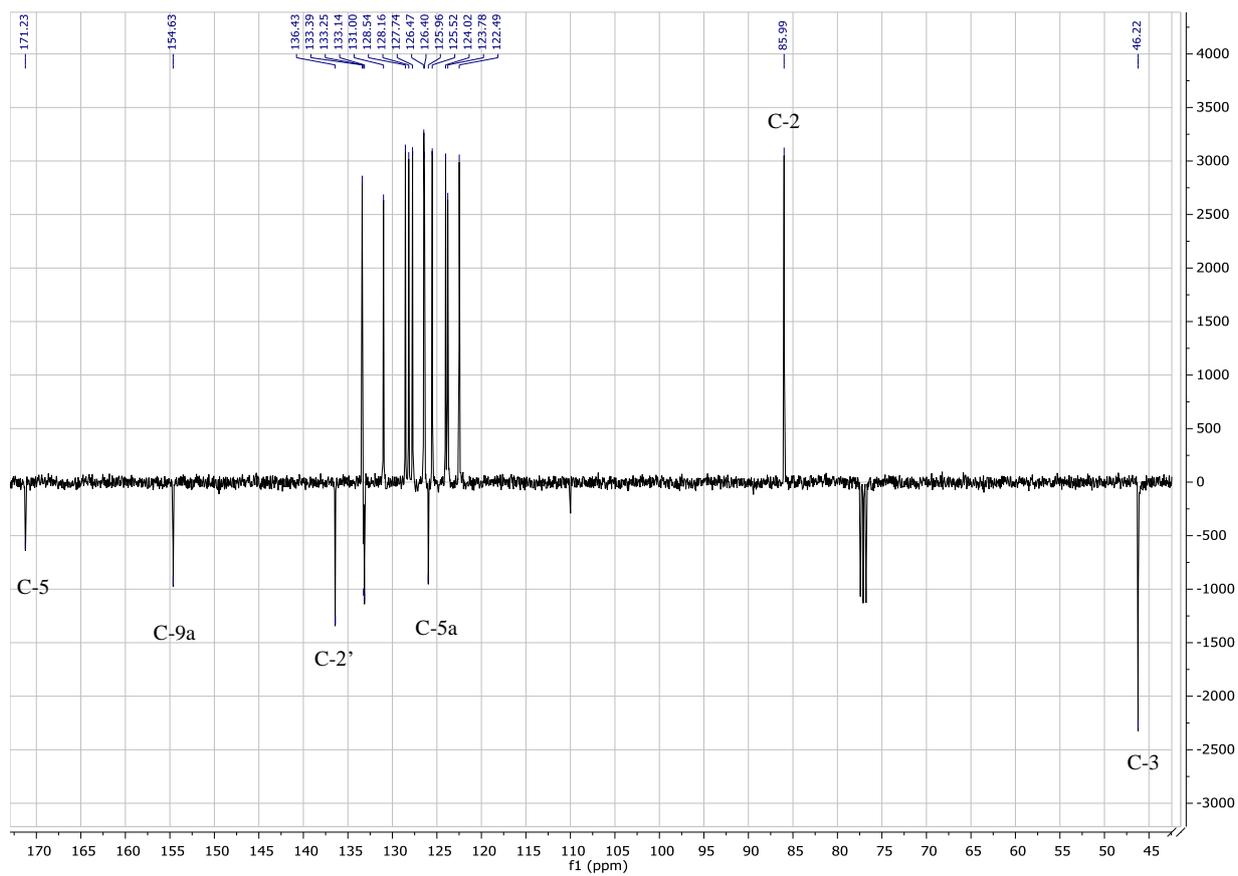
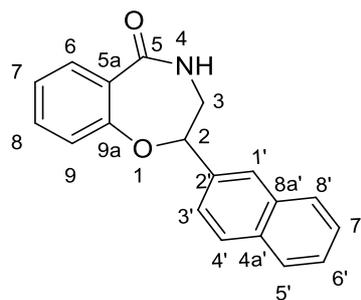


Figure S30. J-modulated ^{13}C -NMR spectrum of *rac*-**8c** measured in CDCl_3 (100 MHz)

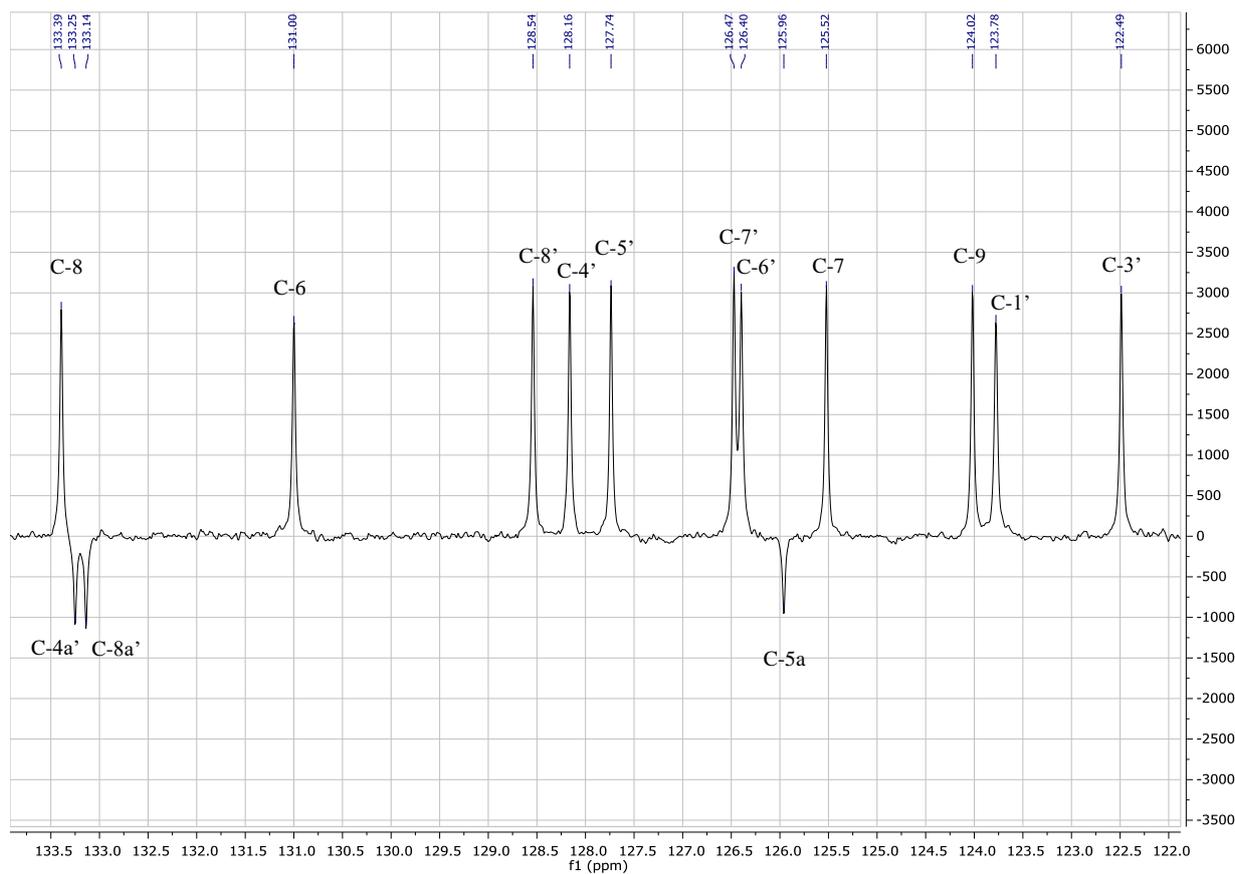
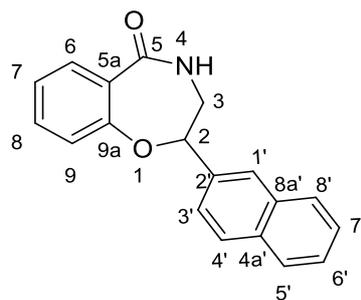


Figure S31 J-modulated ^{13}C -NMR spectrum of *rac*-**8c** measured in CDCl_3 (100 MHz)

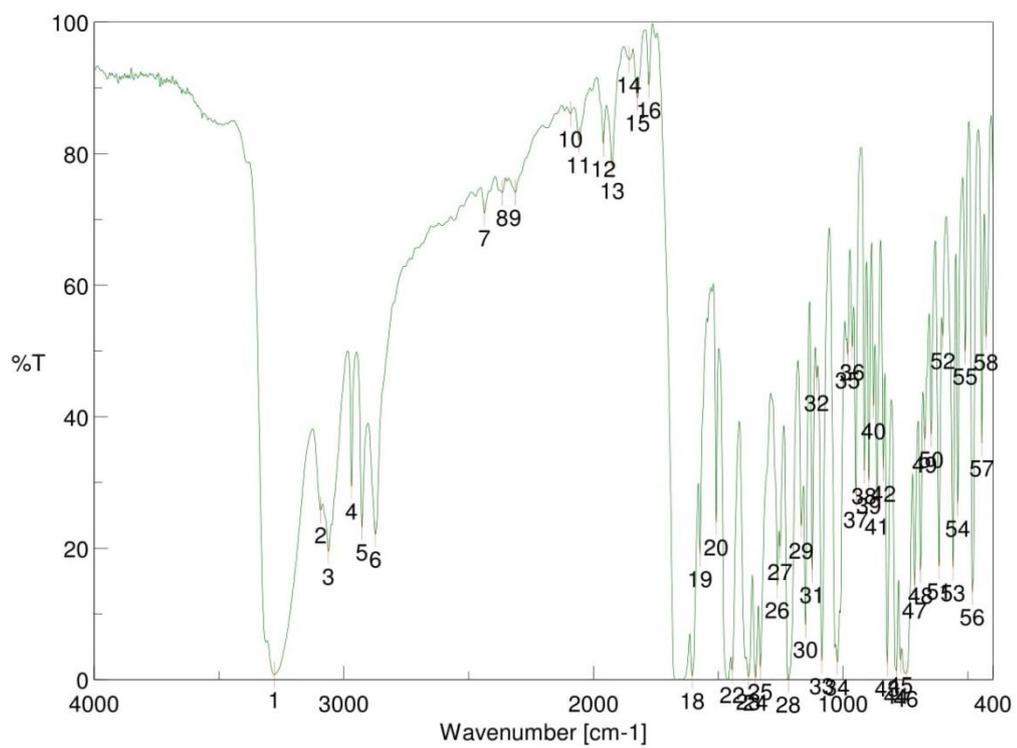
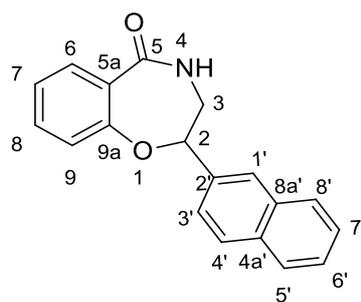


Figure S32 IR spectrum of *rac-8c* recorded as KBr disc

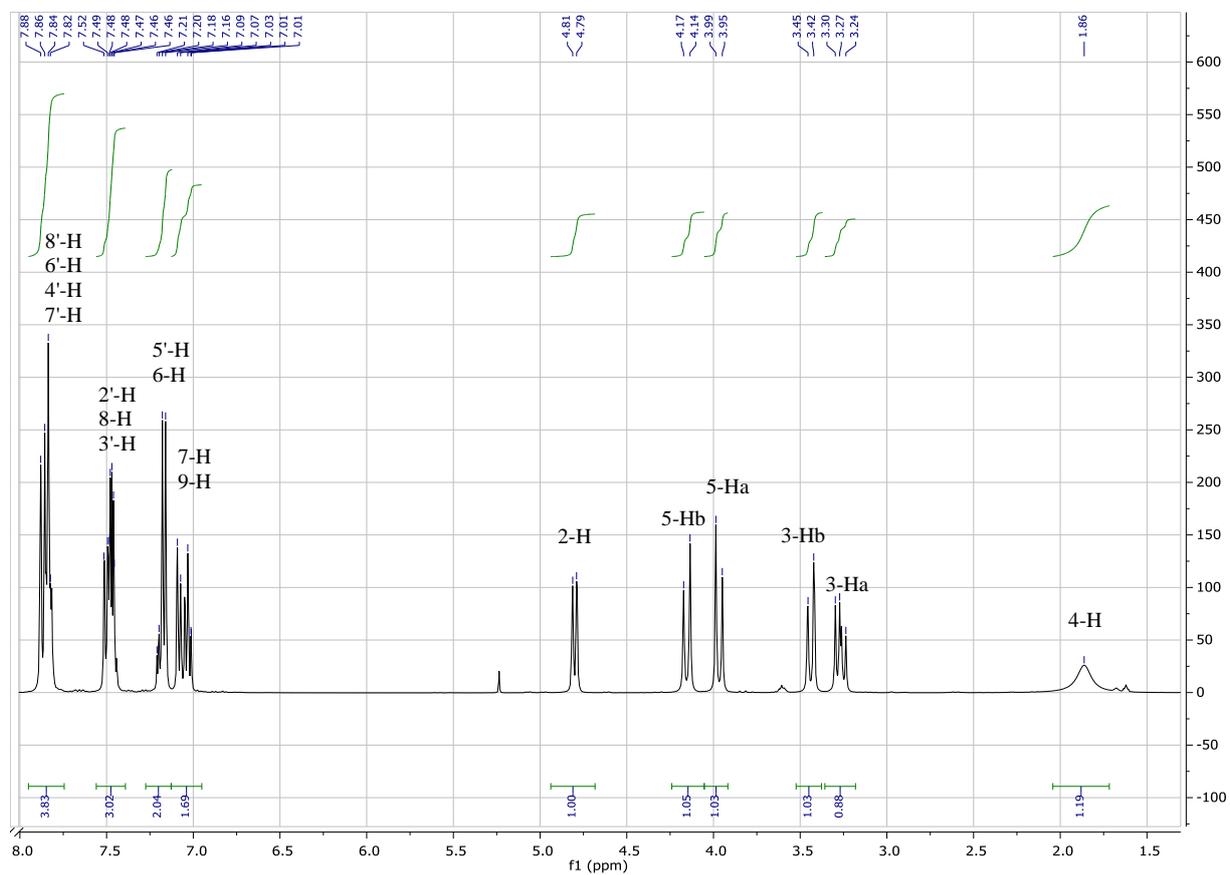
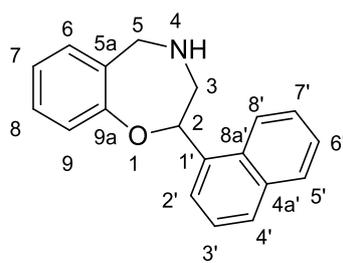


Figure S33. ¹H-NMR spectrum of *rac-9b* measured in CDCl₃ (400 MHz)

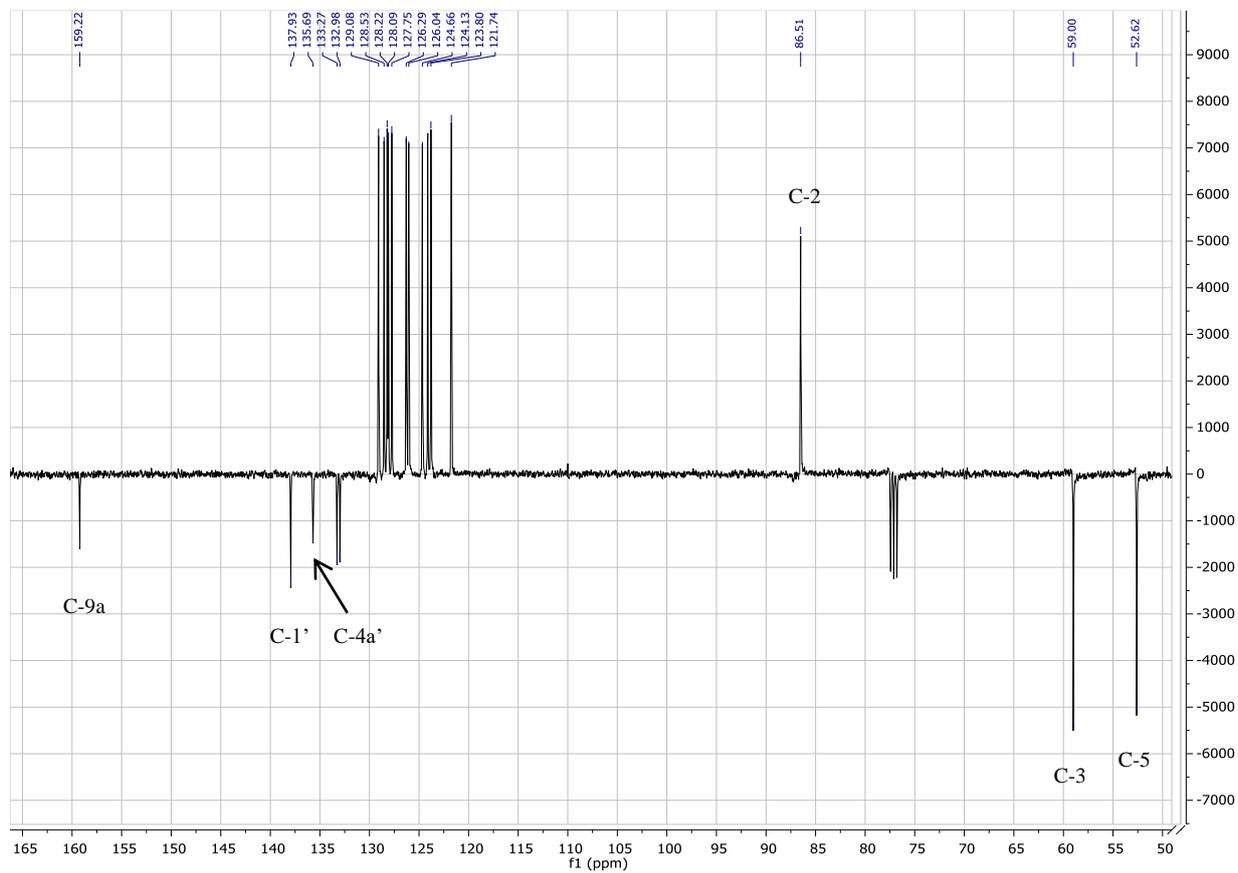
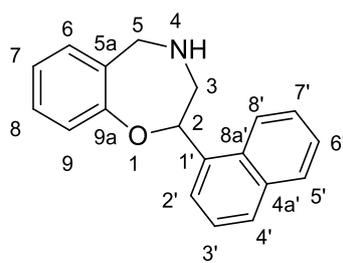


Figure S34. J-modulated ^{13}C -NMR spectrum of *rac*-**9b** measured in CDCl_3 (100 MHz)

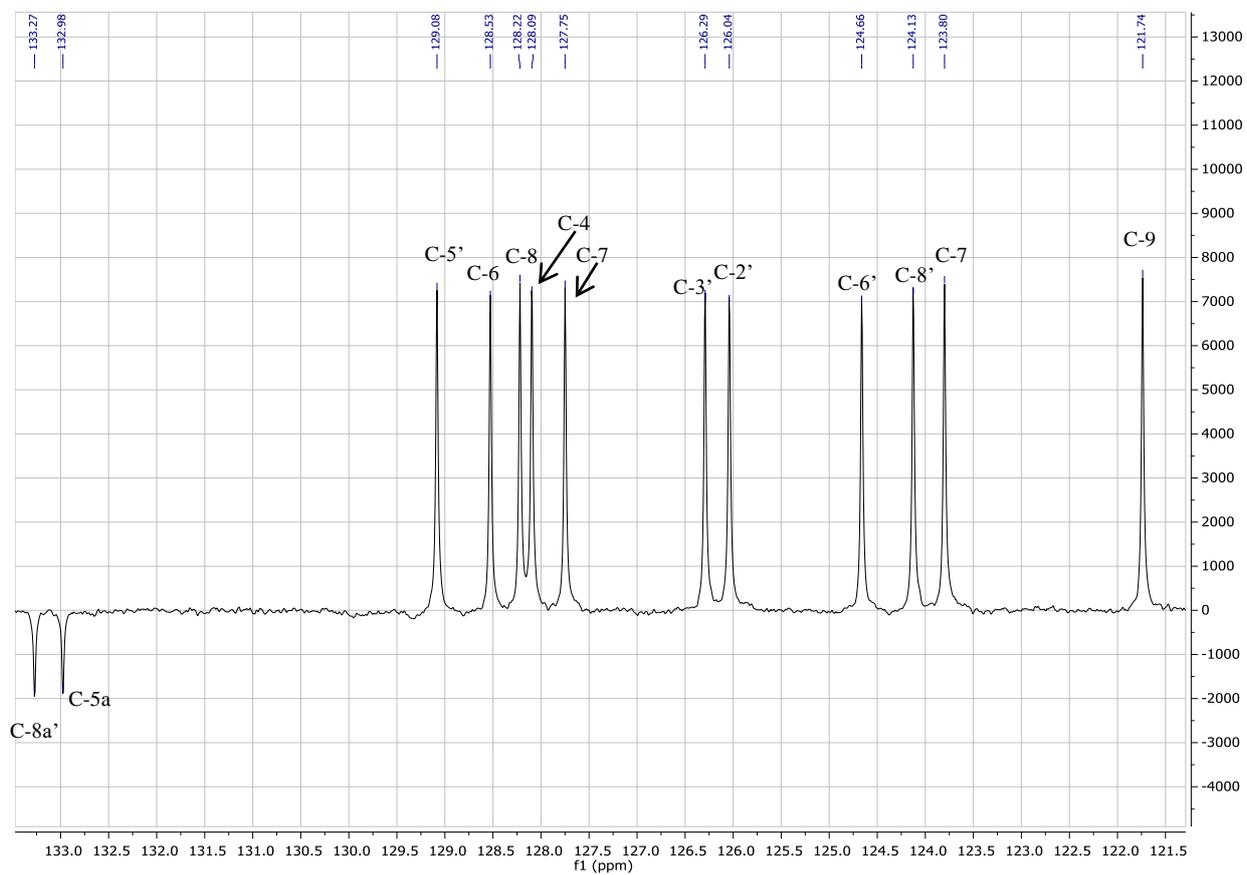
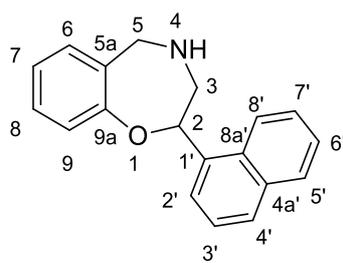


Figure S35. J-modulated ^{13}C -NMR spectrum of *rac*-**9b** measured in CDCl_3 (100 MHz)

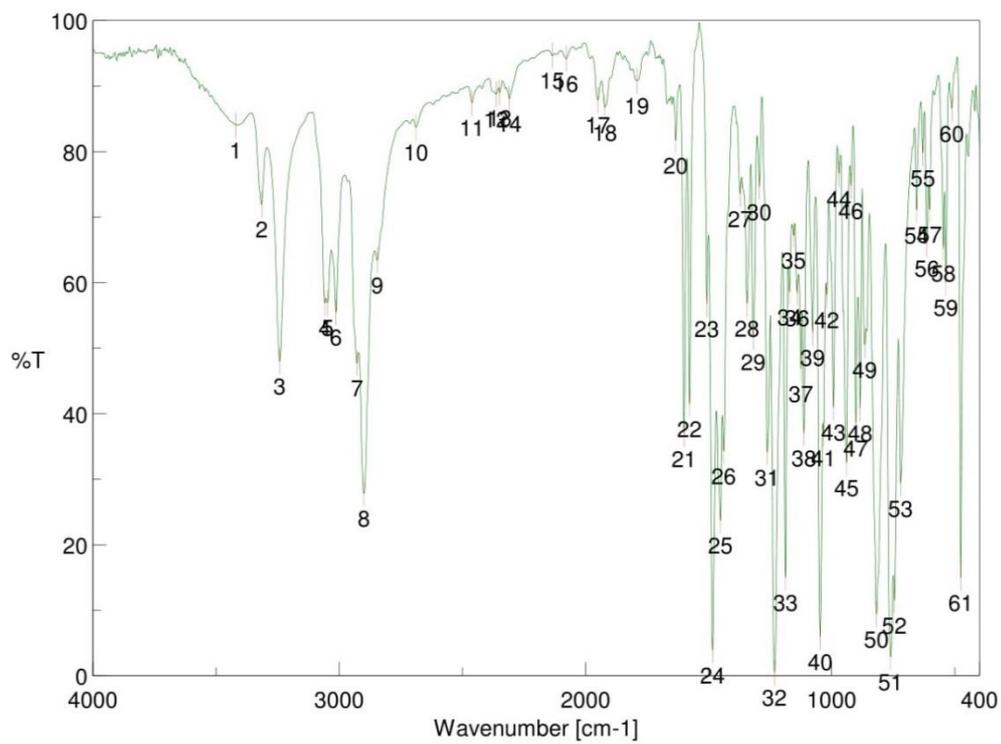
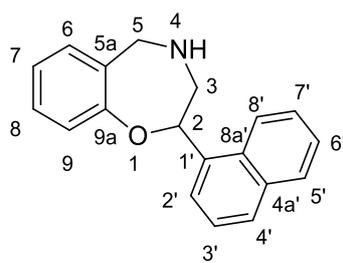


Figure S36. IR spectrum of *rac-9b* recorded as KBr disc

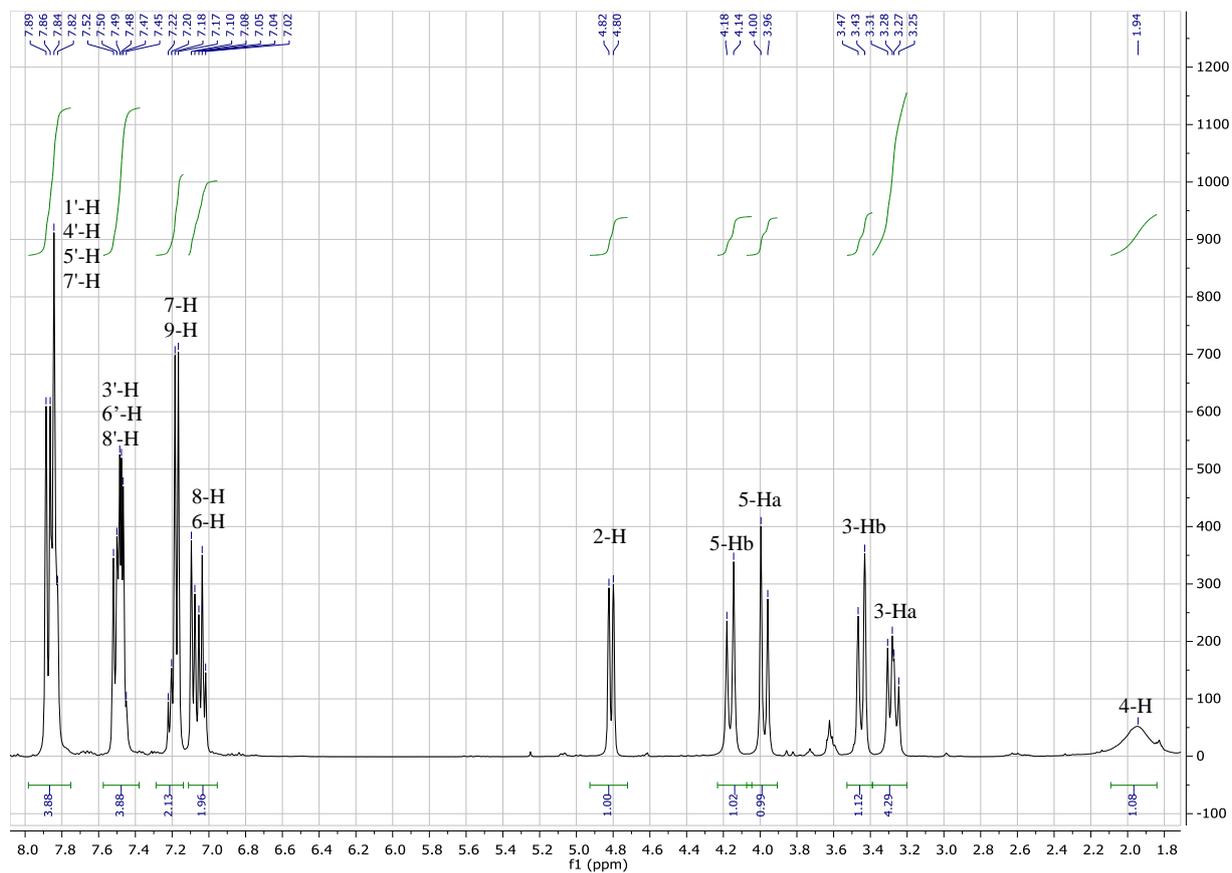
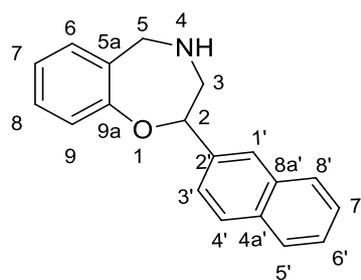


Figure S37. $^1\text{H-NMR}$ spectrum of *rac-9c* measured in CDCl_3 (400 MHz)

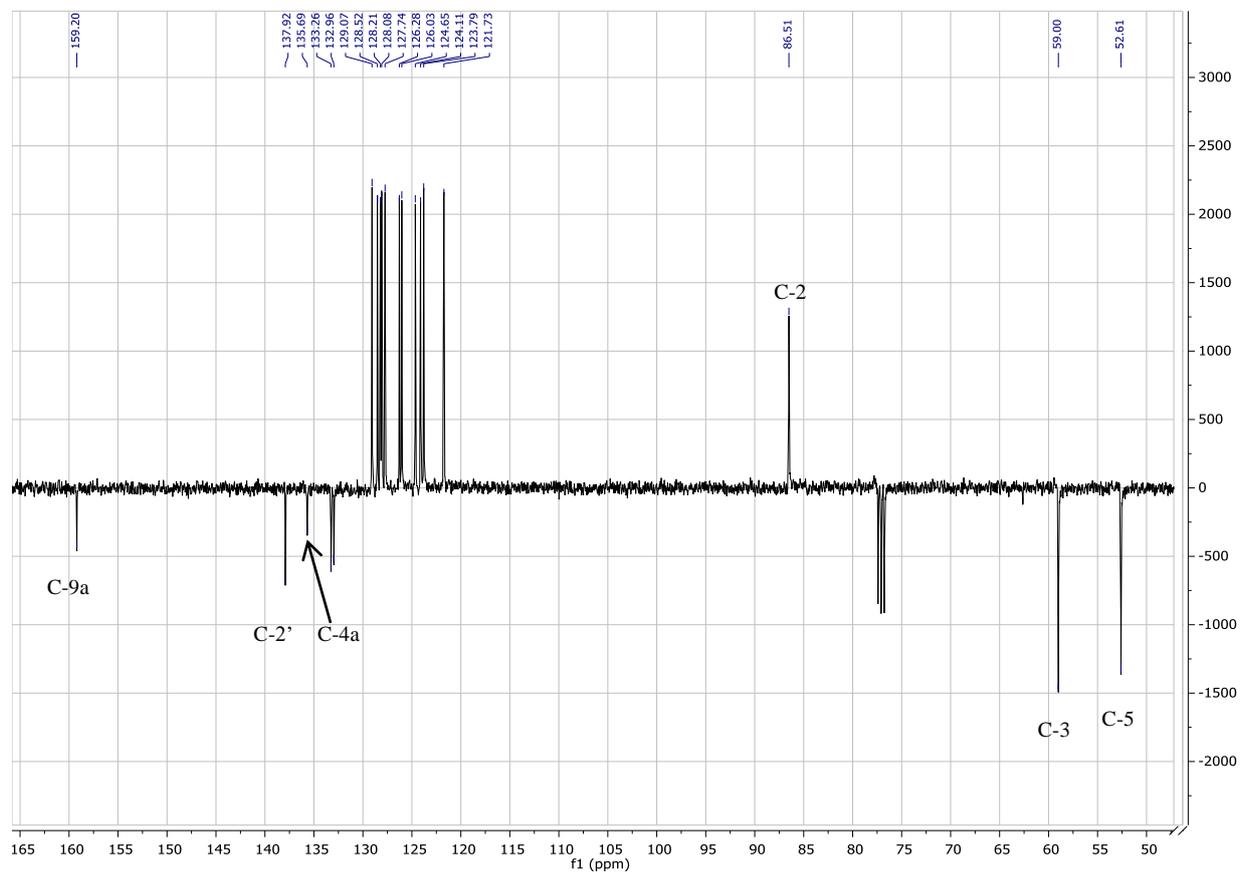
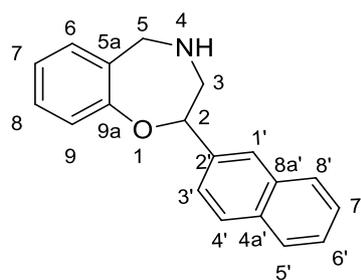


Figure S38. J-modulated ^{13}C -NMR spectrum of *rac-9c* measured in CDCl_3 (100 MHz)

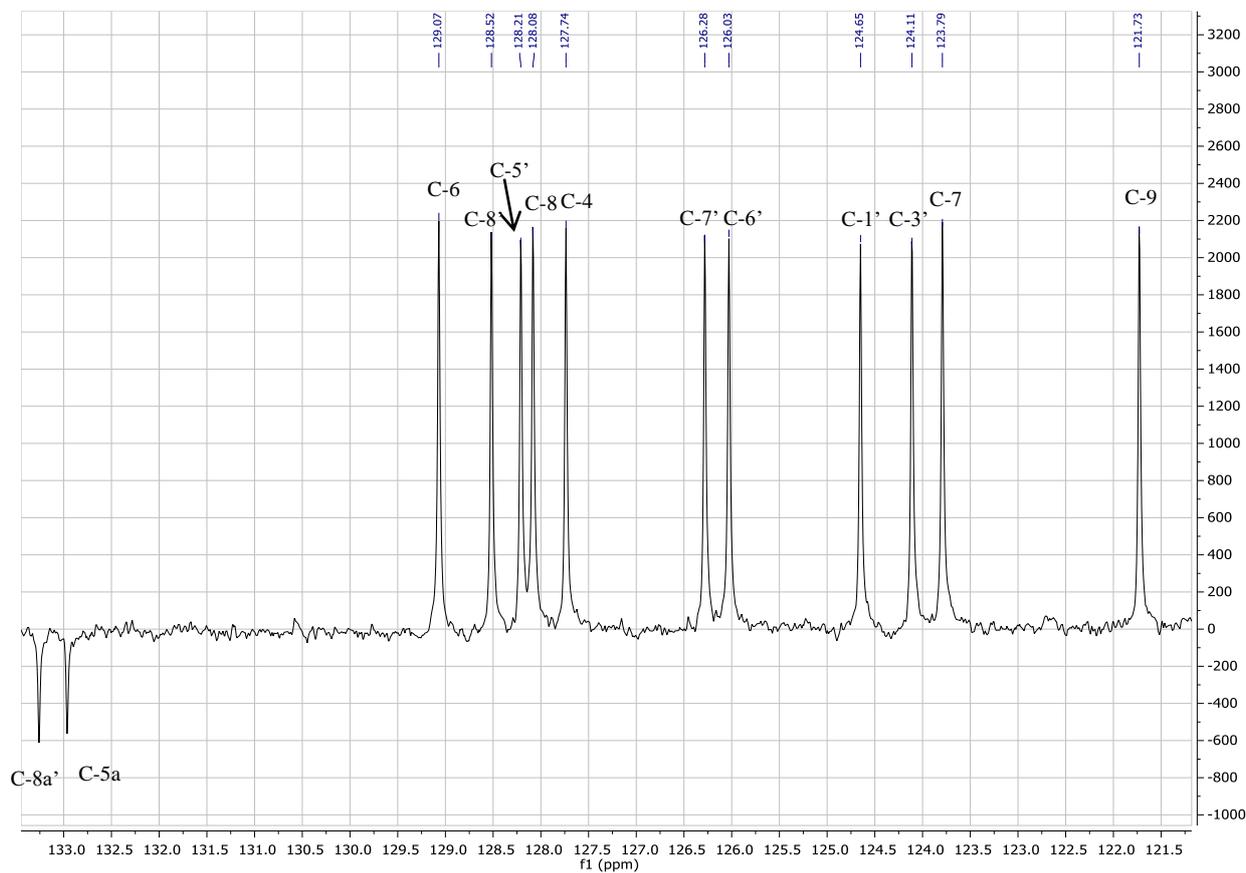
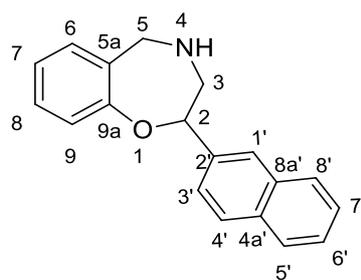


Figure S39. J-modulated ¹³C-NMR spectrum of *rac*-**9c** measured in CDCl₃ (100 MHz)

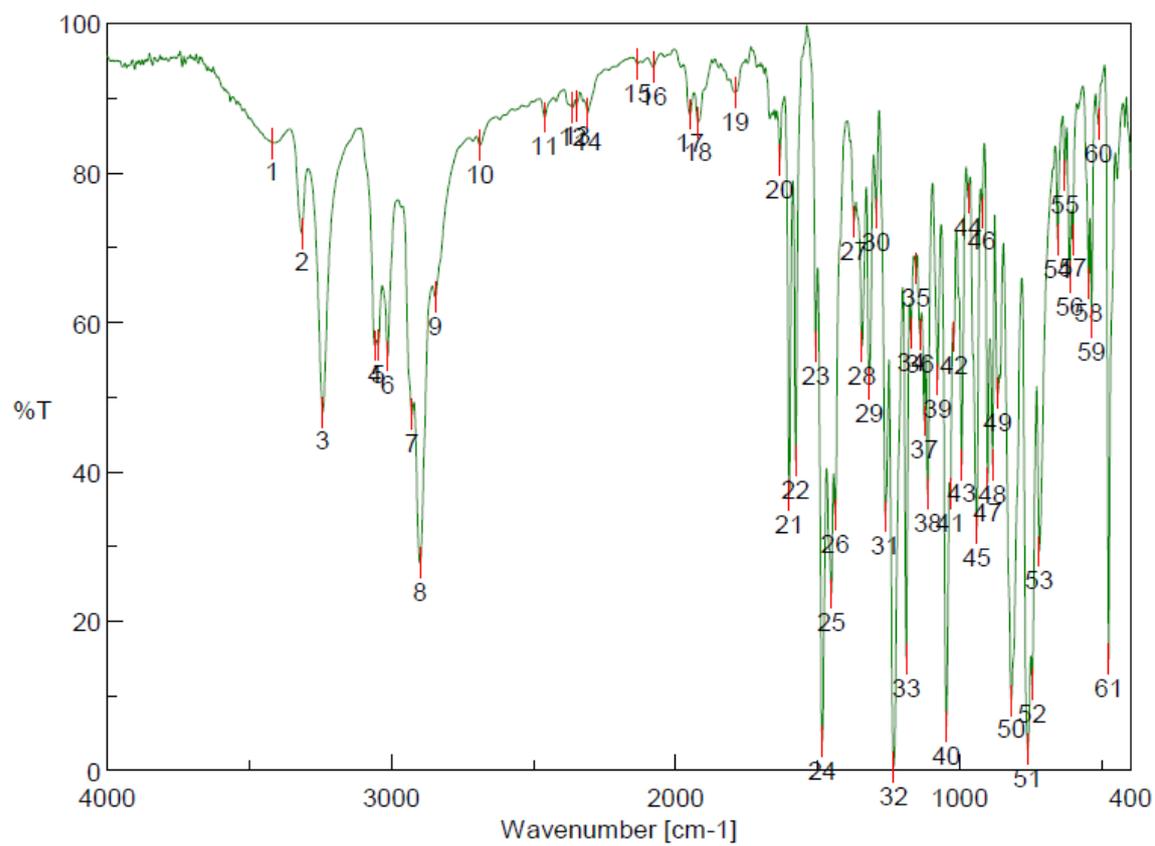
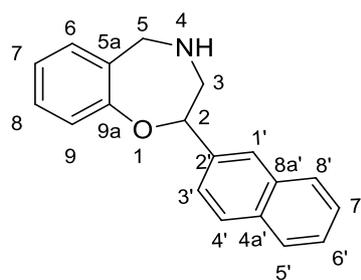


Figure S40. IR spectrum of *rac-9c* recorded as KBr disc

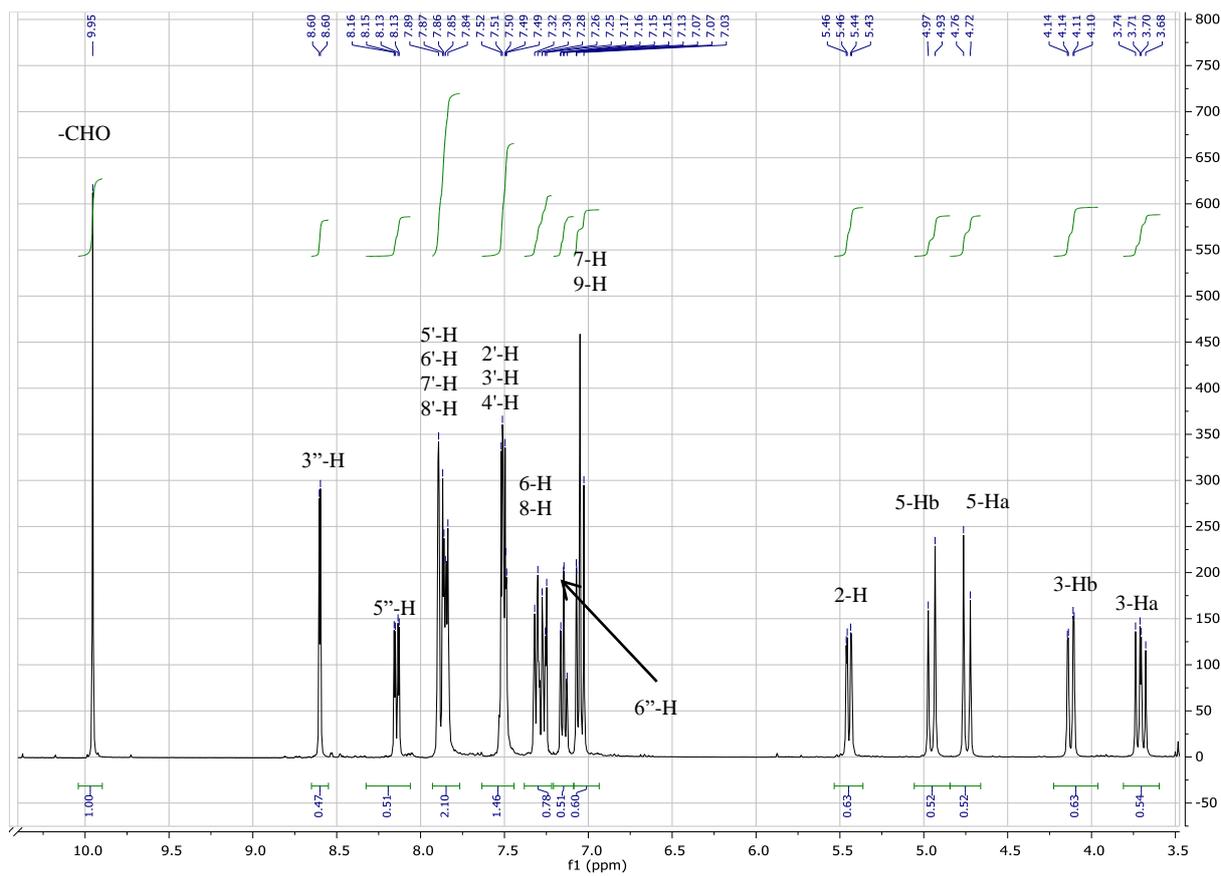
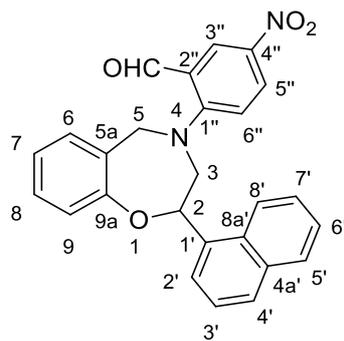


Figure S41. $^1\text{H-NMR}$ spectrum of *rac-1b* measured in CDCl_3 (400 MHz)

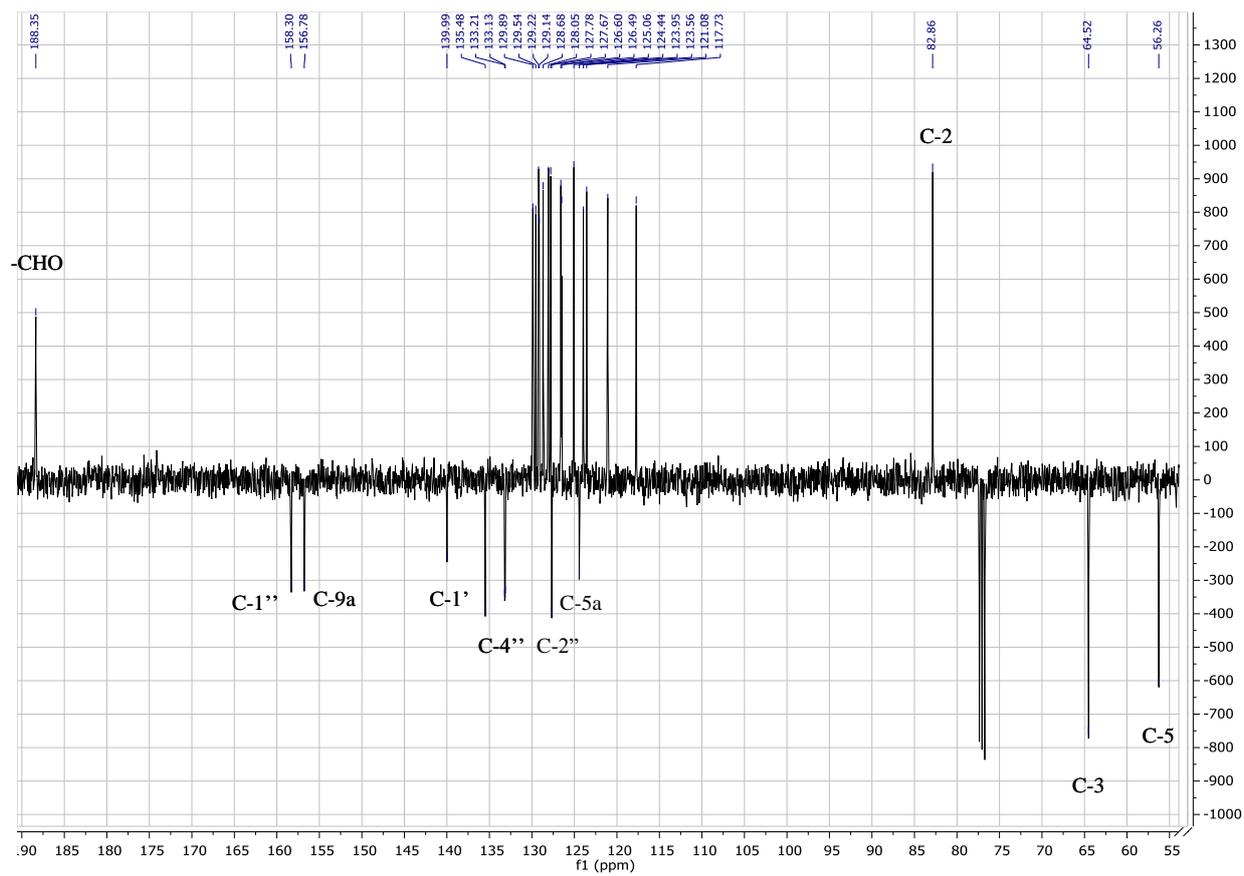
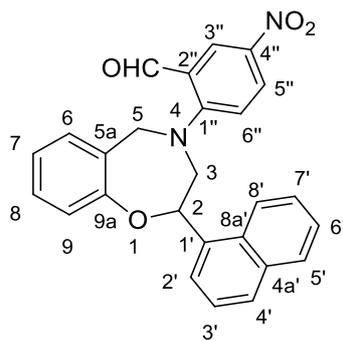


Figure S42. J-modulated ^{13}C -NMR spectrum of *rac*-**1b** measured in CDCl_3 (100 MHz)

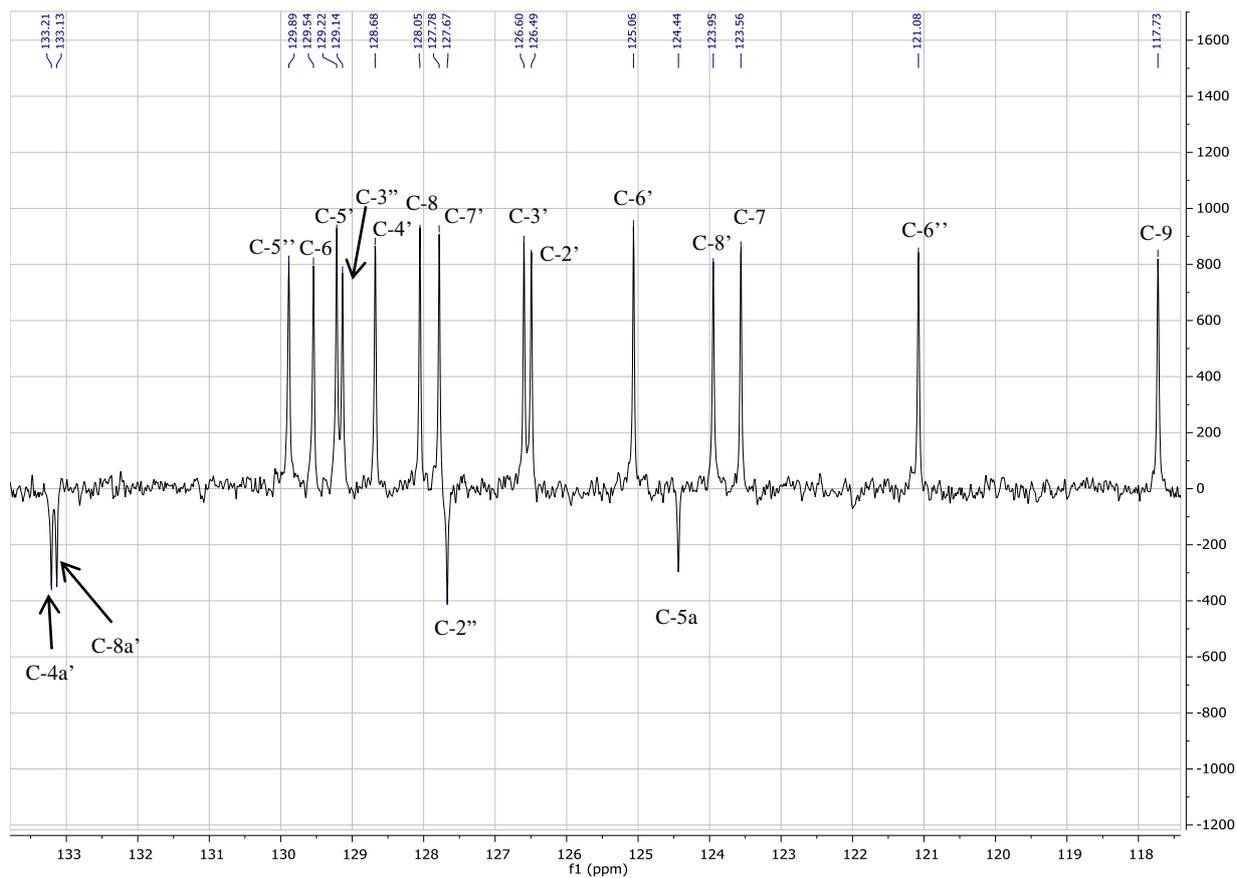
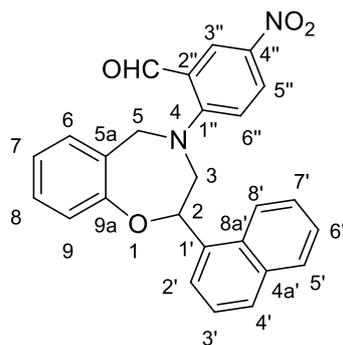


Figure S43. J-modulated ^{13}C -NMR spectrum of *rac*-**1b** measured in CDCl_3 (100 MHz)

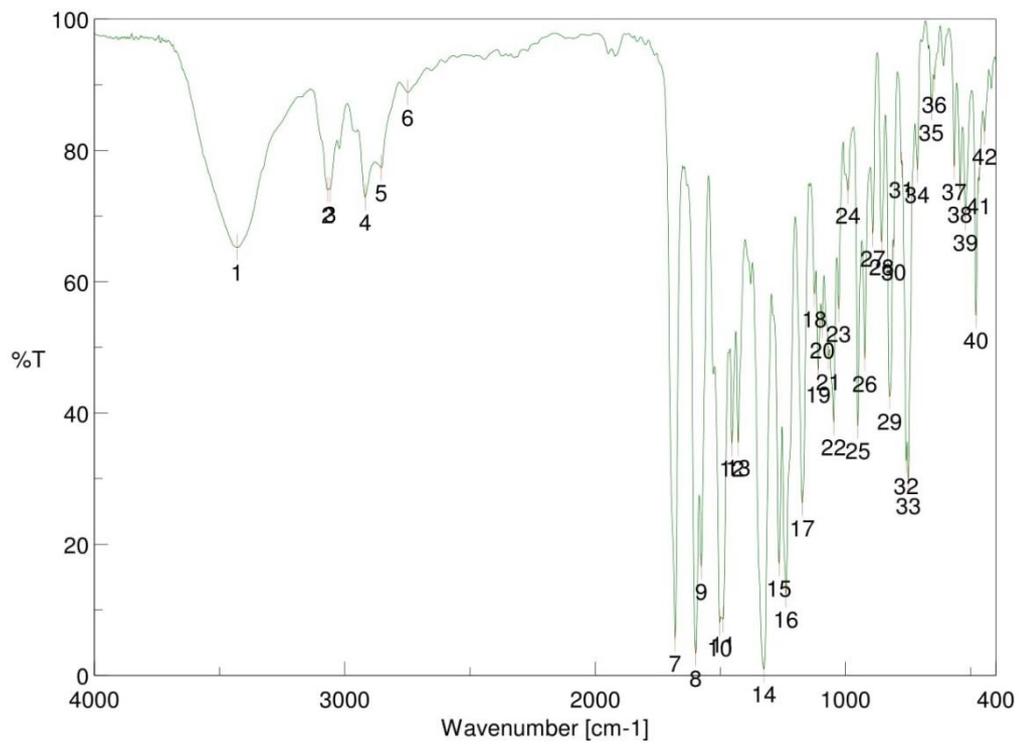
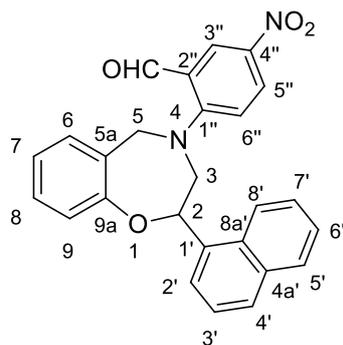


Figure S44. IR spectrum of *rac*-**1b** recorded as KBr disc

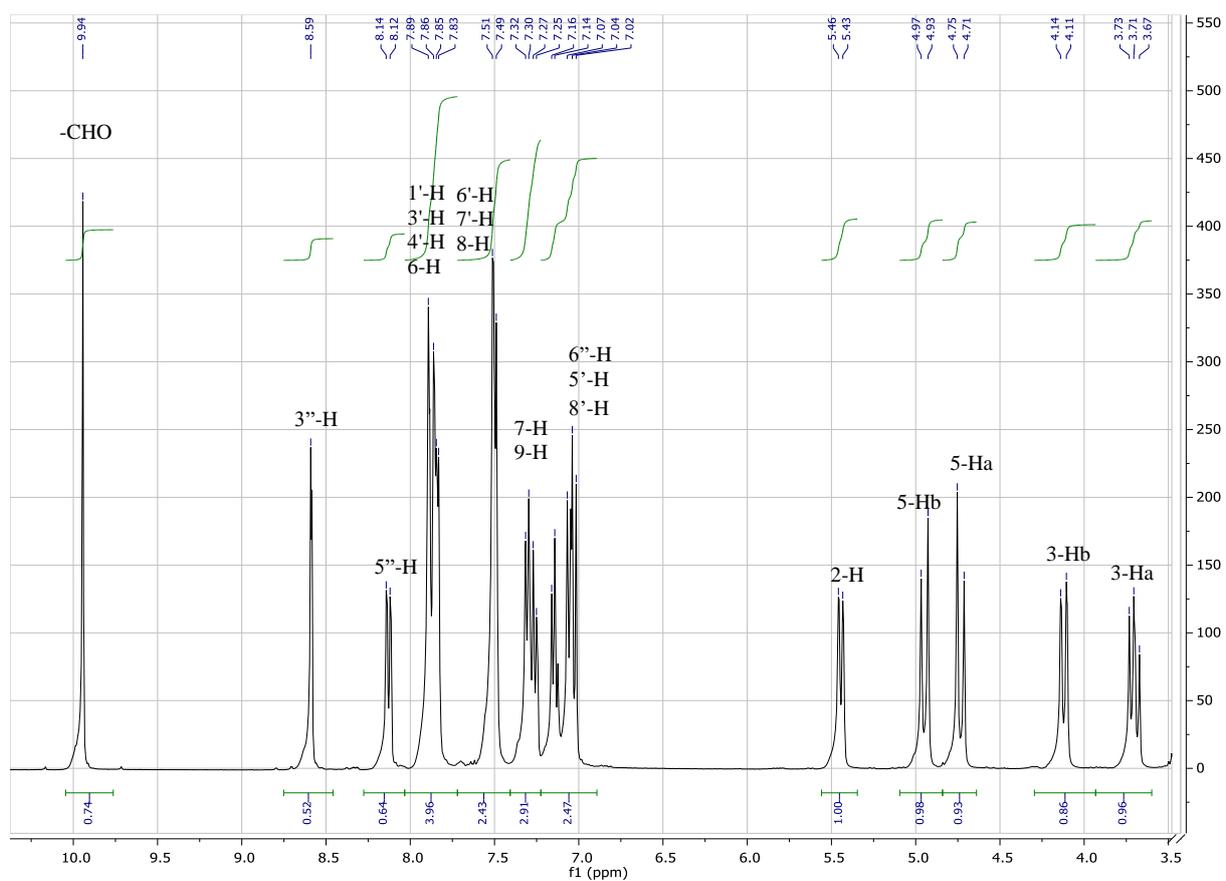
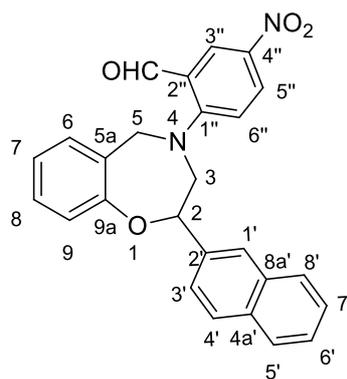


Figure S45. $^1\text{H-NMR}$ spectrum of *rac-1c* measured in CDCl_3 (400 MHz)

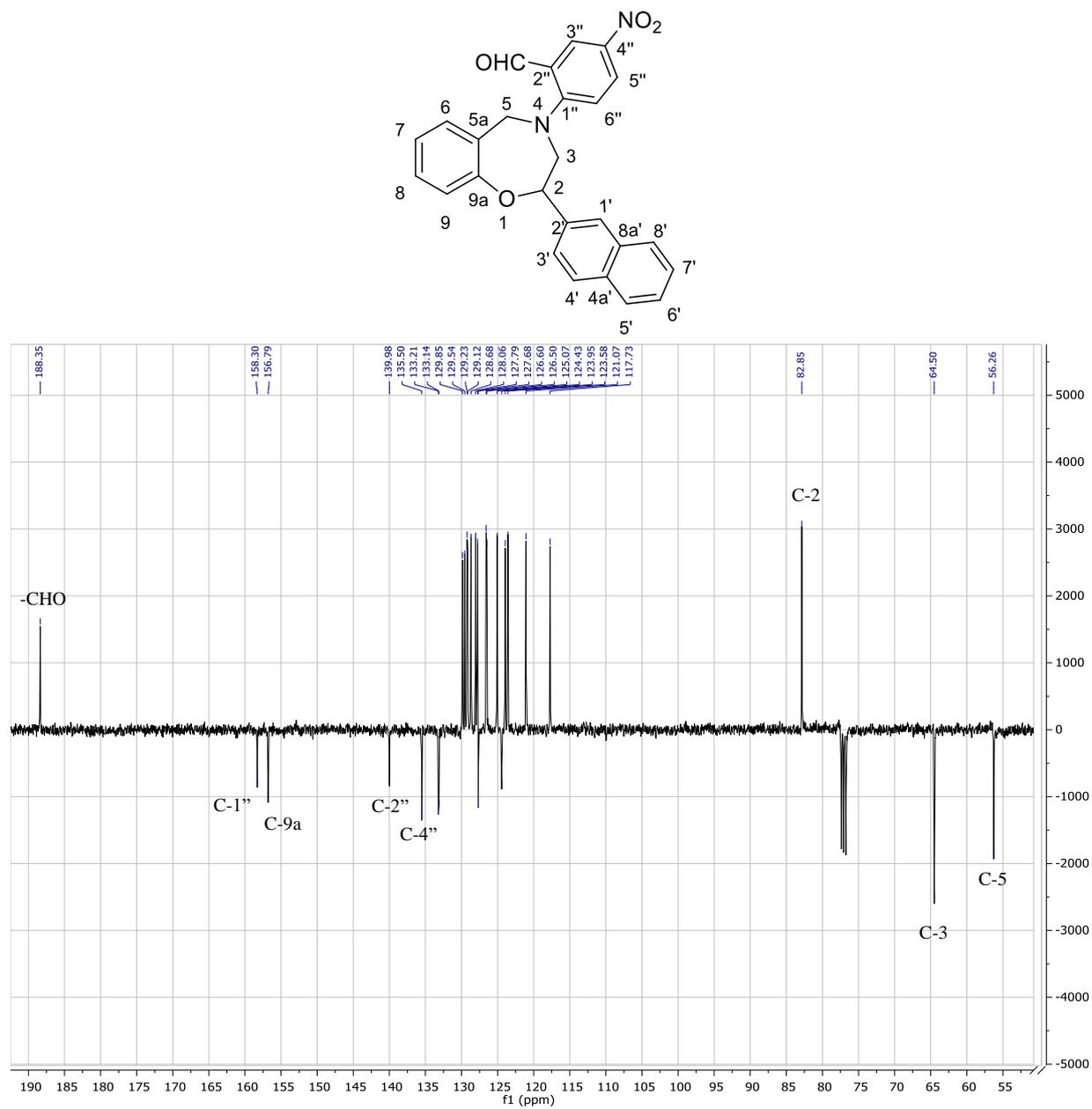


Figure S46. J-modulated ^{13}C -NMR spectrum of *rac-1c* measured in CDCl_3 (100 MHz)

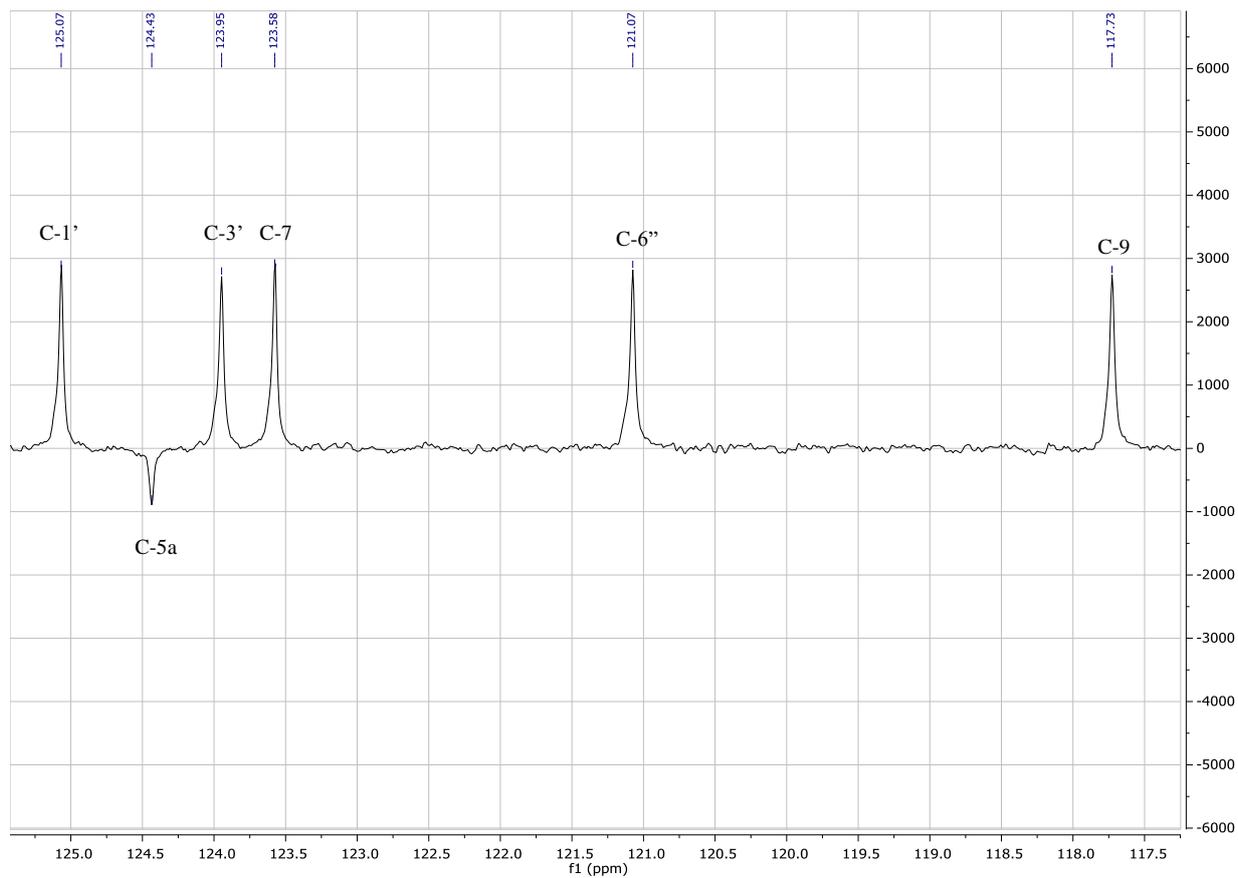
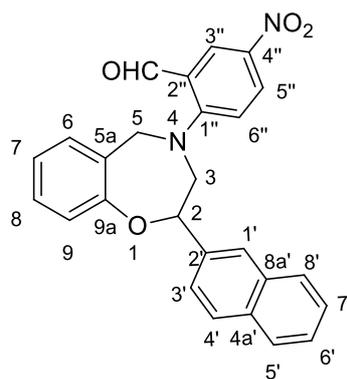


Figure S47. J-modulated ^{13}C -NMR spectrum of *rac*-**1c** measured in CDCl_3 (100 MHz)

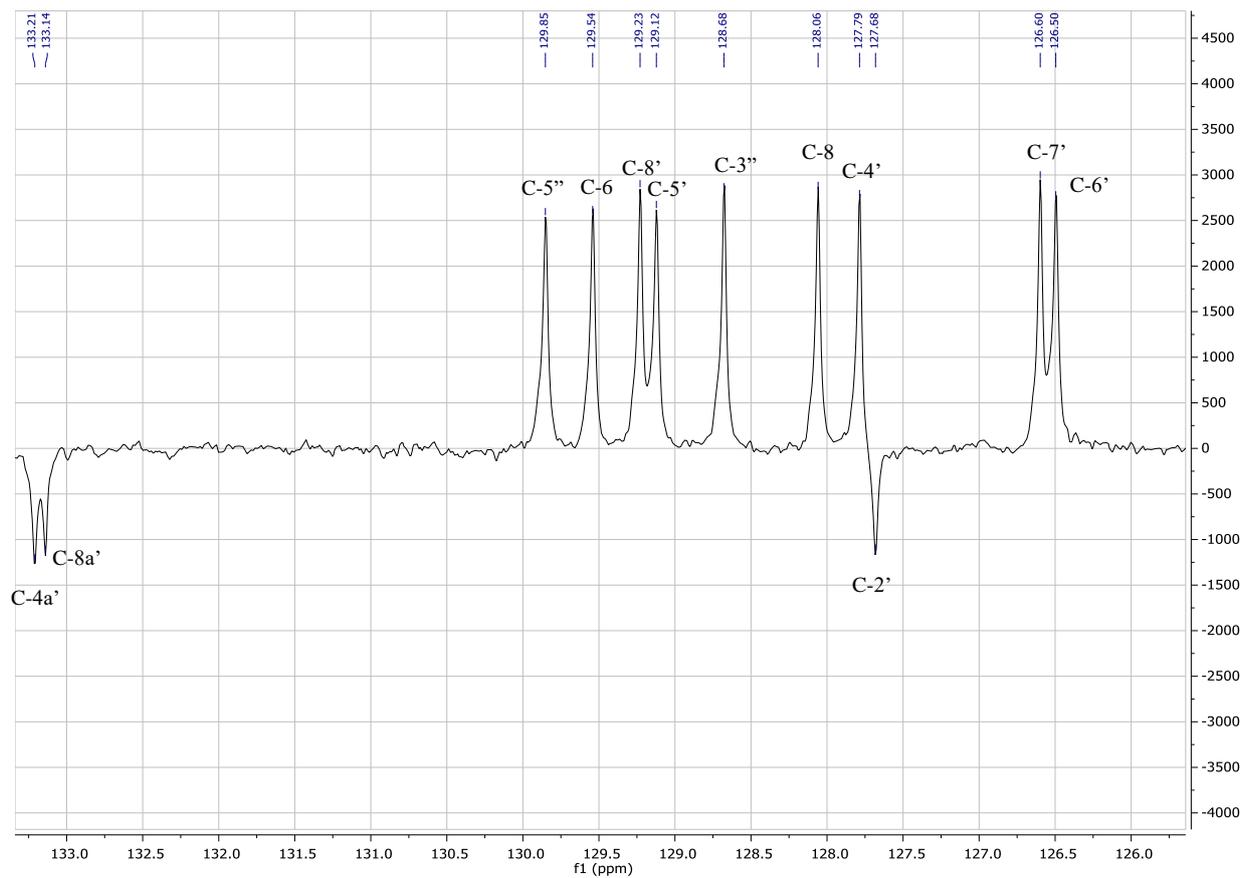
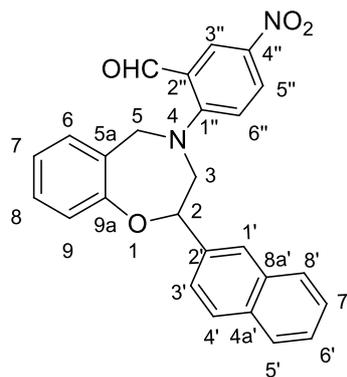


Figure S48. J-modulated ^{13}C -NMR spectrum of *rac*-**1c** measured in CDCl_3 (100 MHz)

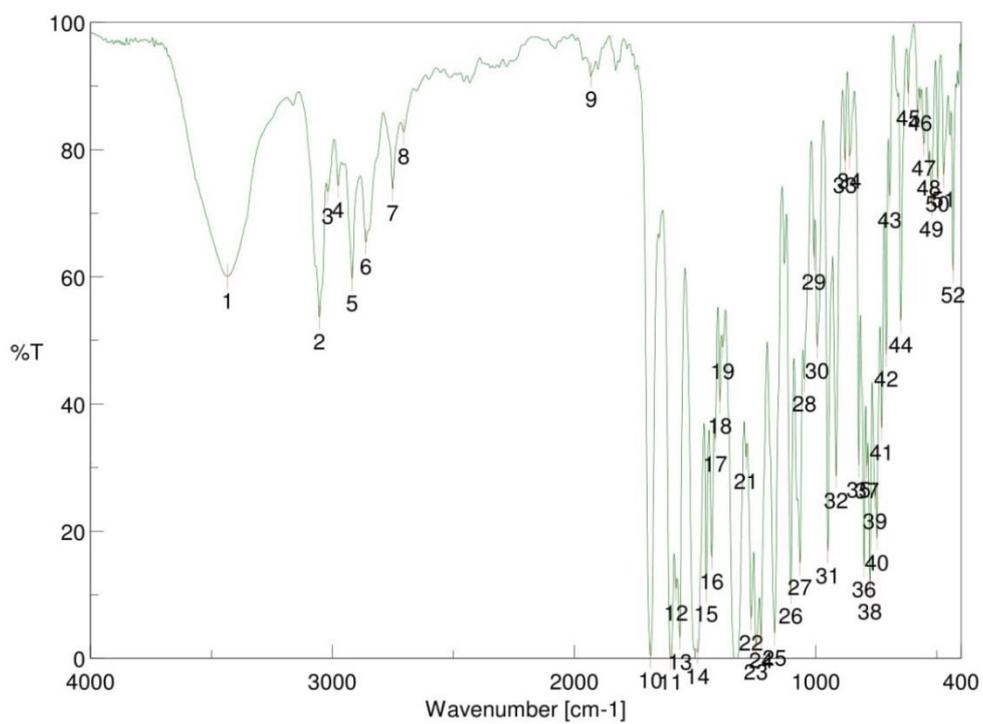
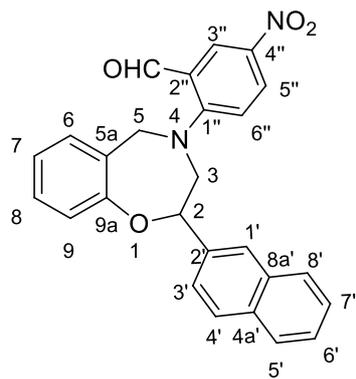


Figure S49. IR spectrum of *rac-1c* recorded as KBr disc

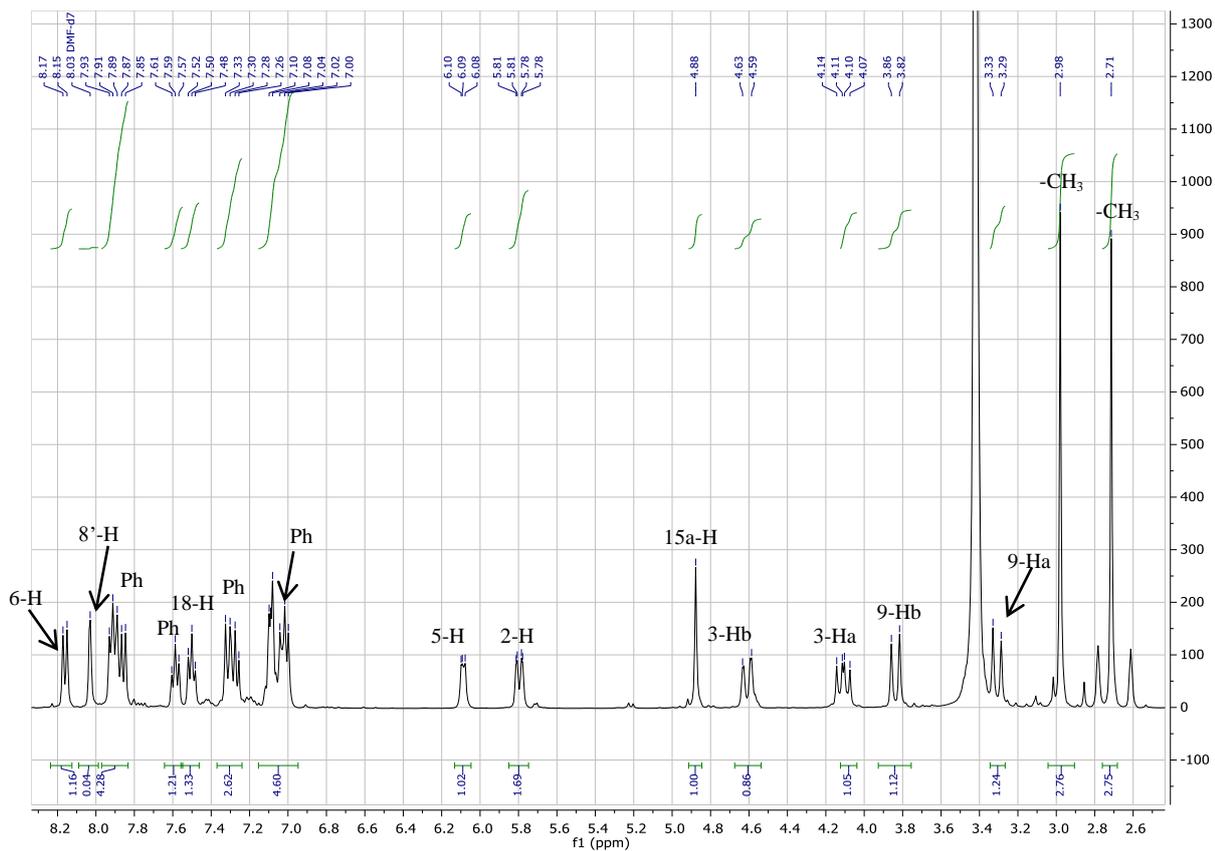
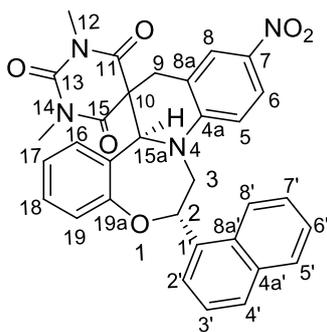


Figure S50. ¹H-NMR spectrum of *rac-10b* measured in DMF-d₇ (400 MHz)

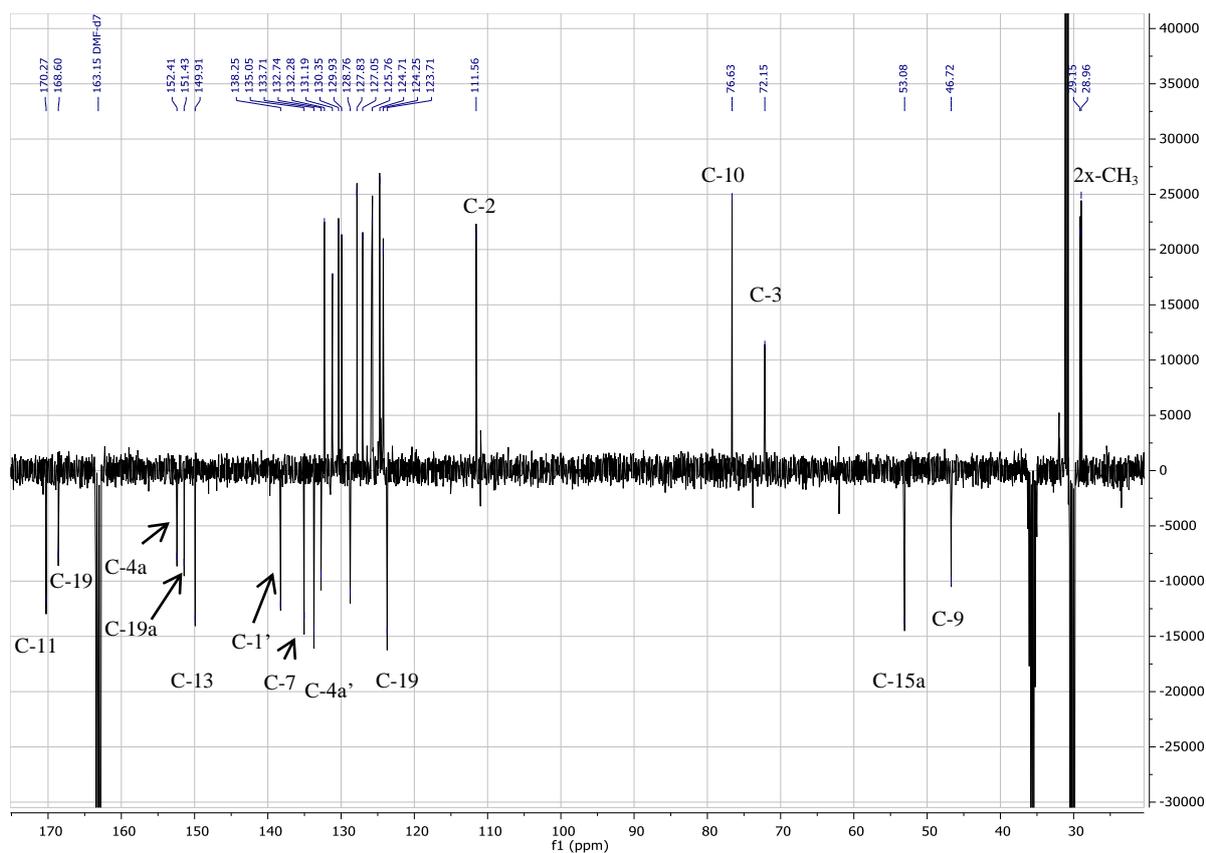
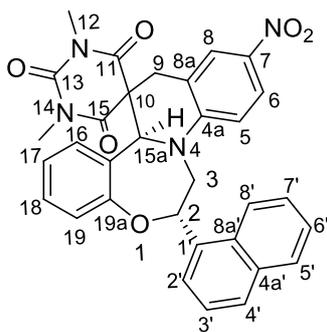


Figure S51. J-modulated ^{13}C -NMR spectrum of *rac*-**10b** measured in DMF-d_7 (100 MHz)

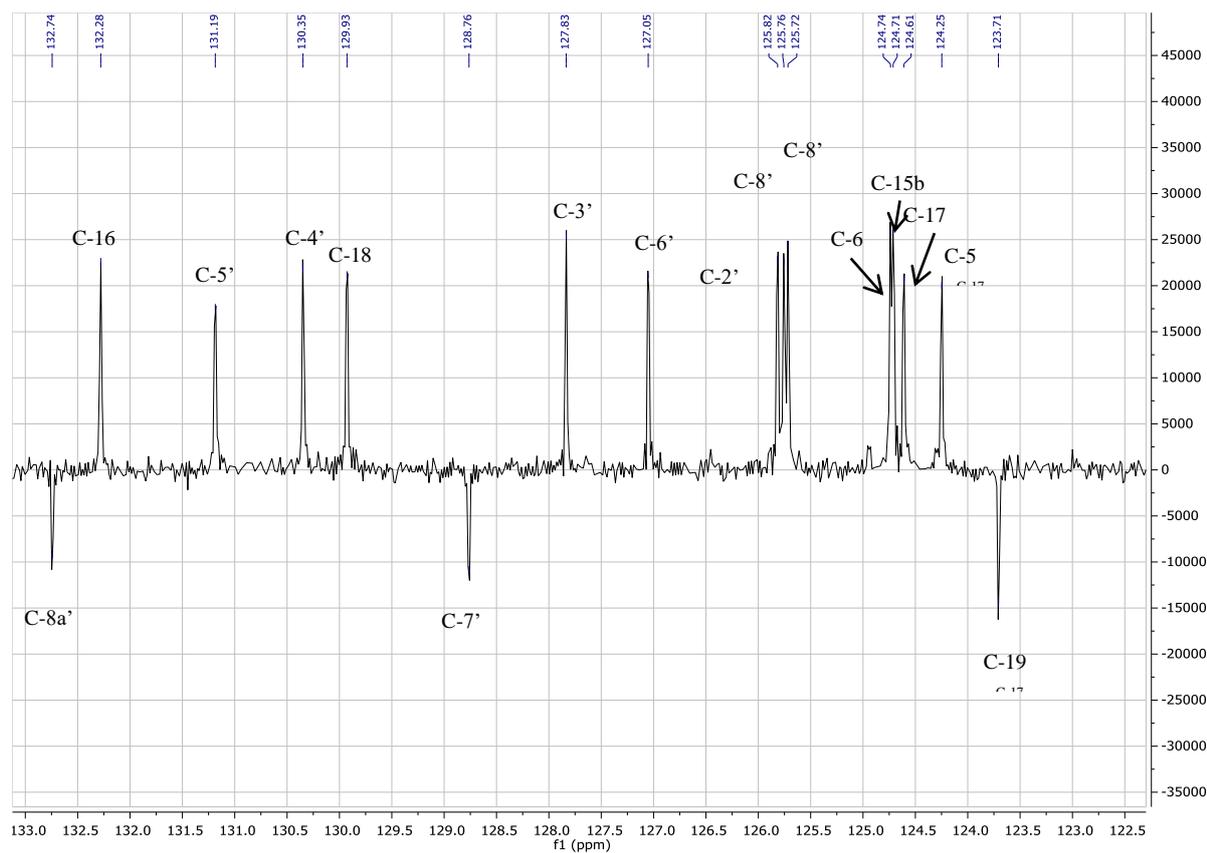
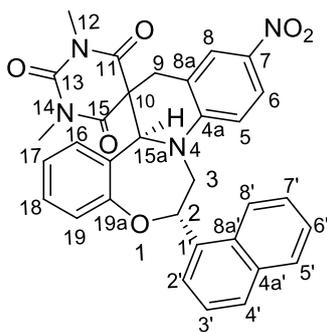


Figure S52. J-modulated ¹³C-NMR spectrum of *rac-10b* measured in DMF-d₇ (100 MHz)

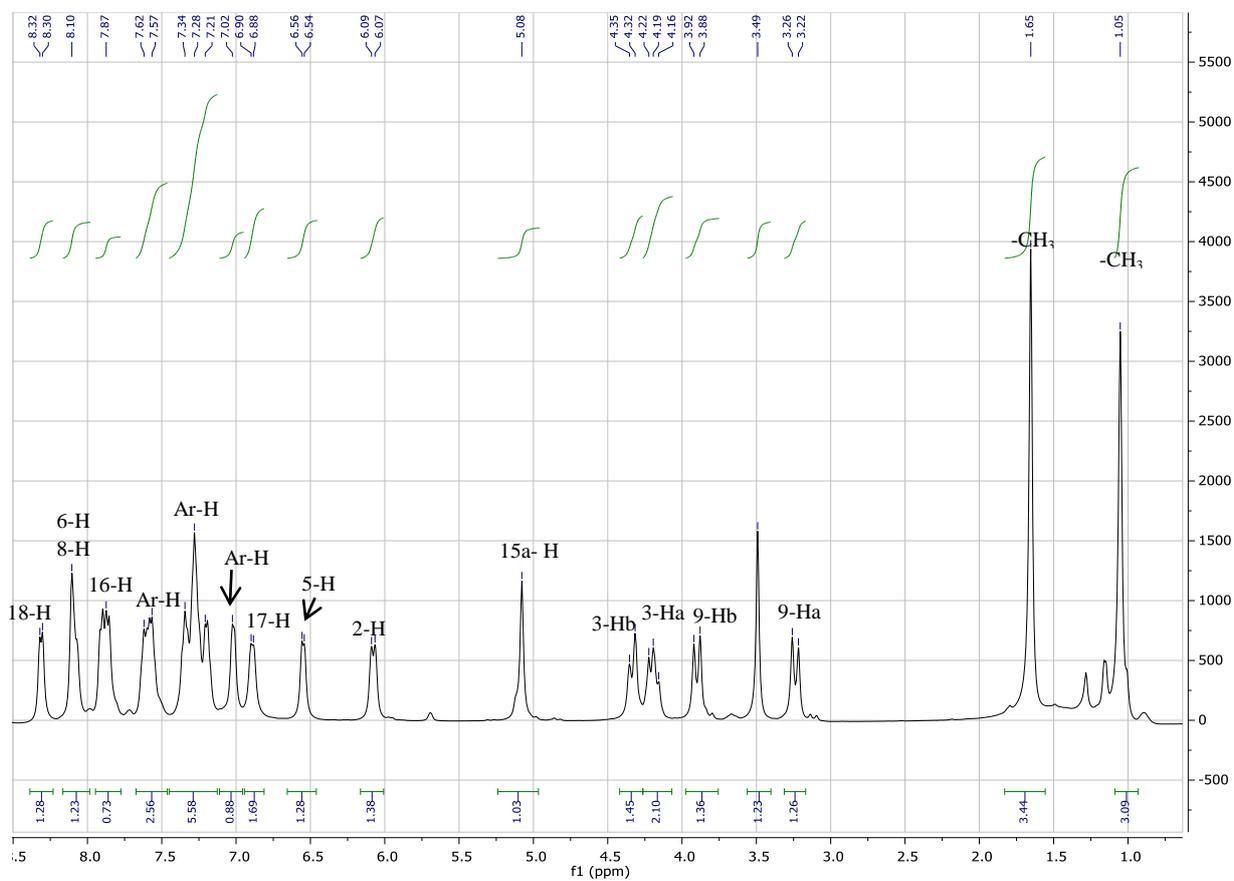
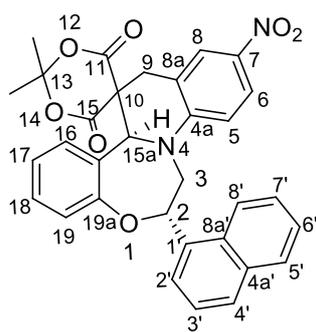


Figure S53. $^1\text{H-NMR}$ spectrum of *rac*-**11b** measured in CDCl_3 (400 MHz)

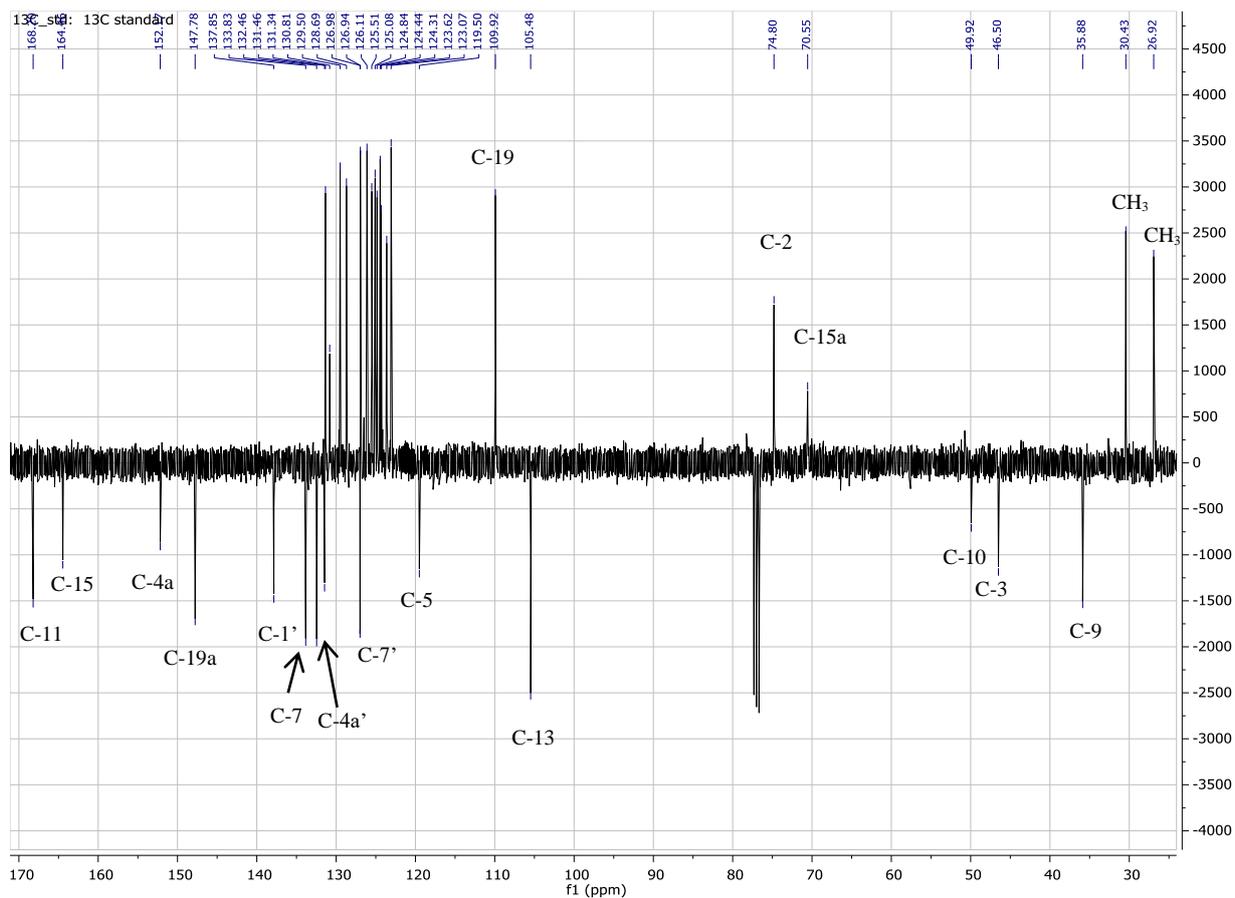
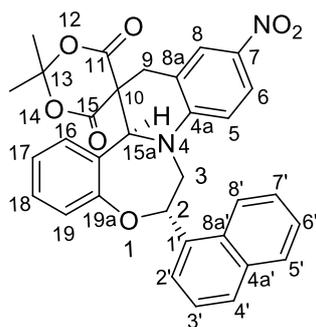


Figure S54. J-modulated ¹³C-NMR spectrum of *rac*-**11b** measured in CDCl₃ (100 MHz)

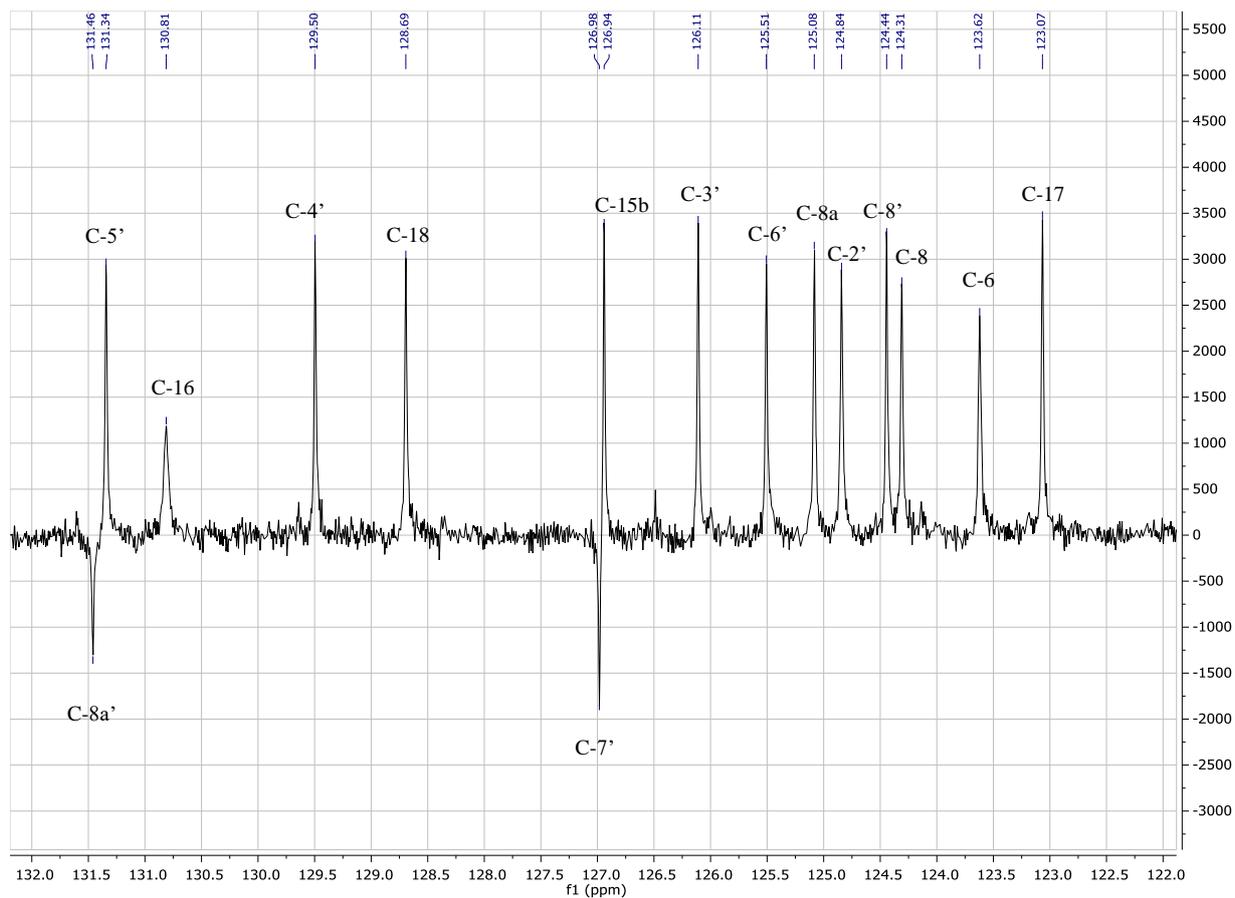
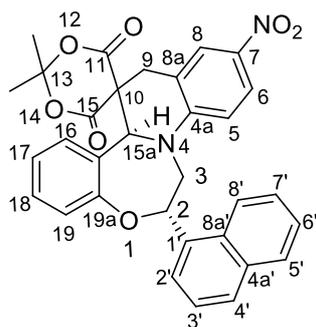


Figure S55. J-modulated ¹³C-NMR spectrum of *rac-11b* measured in CDCl₃ (100 MHz)

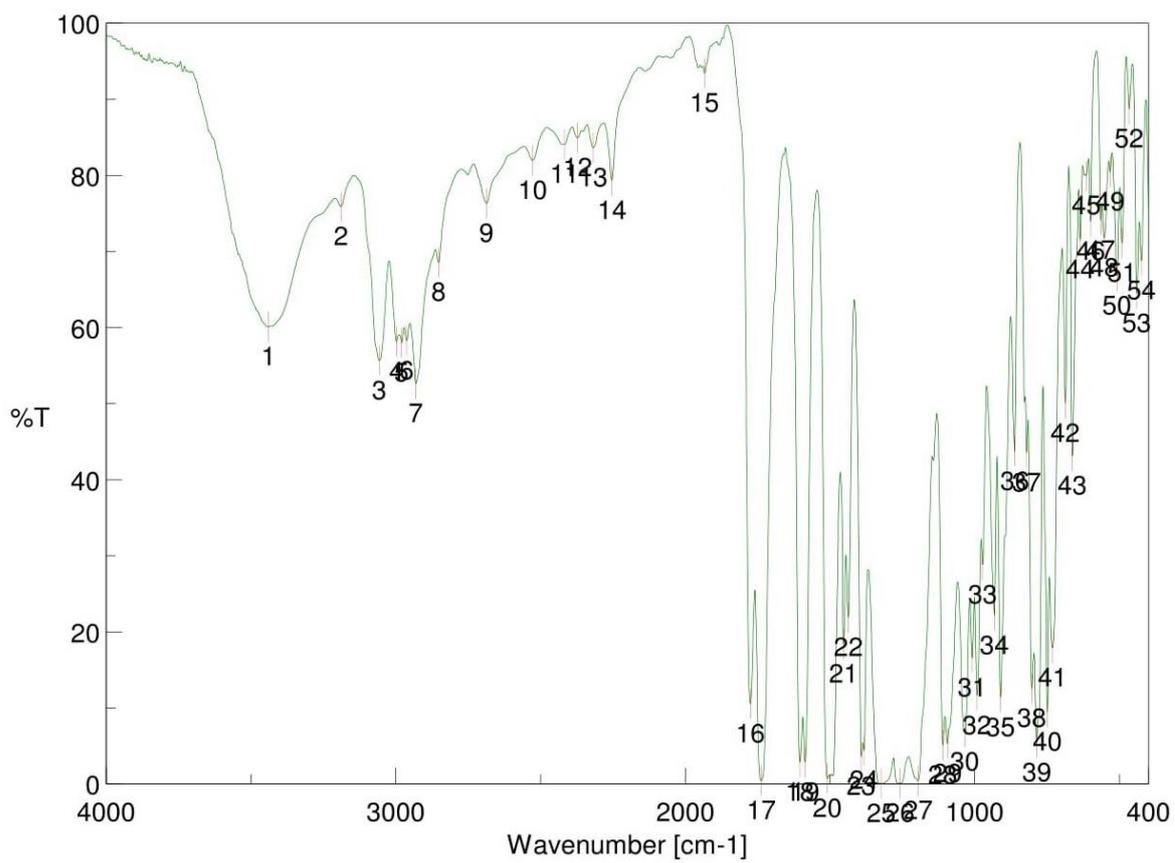
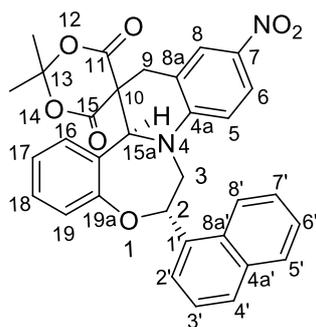


Figure S56. IR spectrum of *rac-11b* recorded as KBr disc

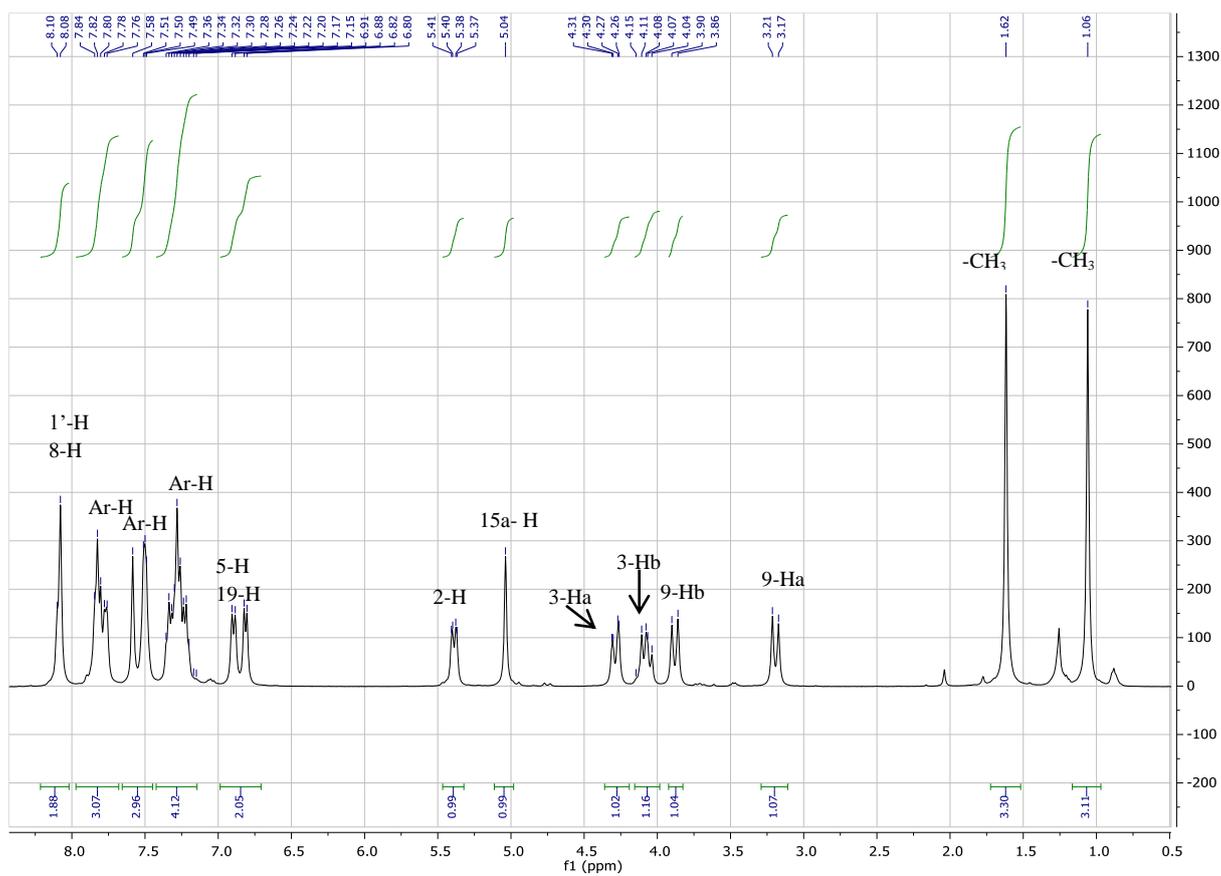
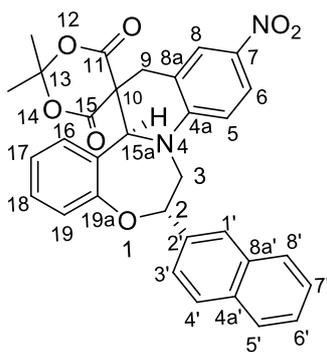


Figure S57. $^1\text{H-NMR}$ spectrum of *rac-11c* measured in CDCl_3 (400 MHz)

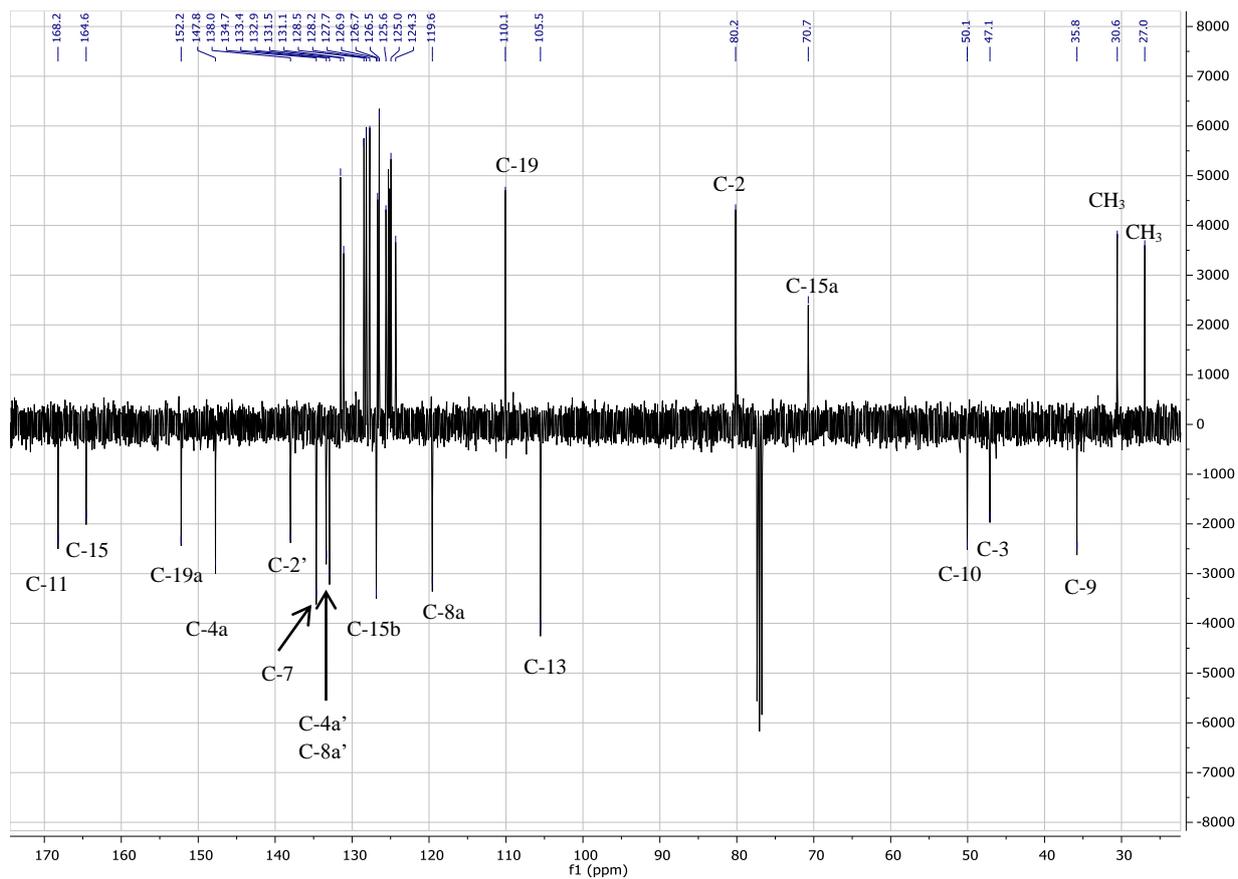
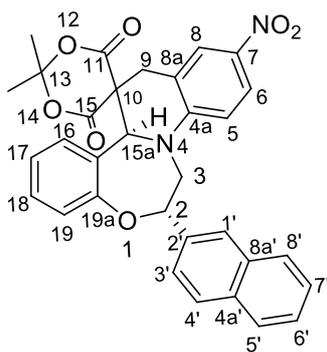


Figure S58. J-modulated ^{13}C -NMR spectrum of *rac*-**11c** measured in CDCl_3 (100 MHz)

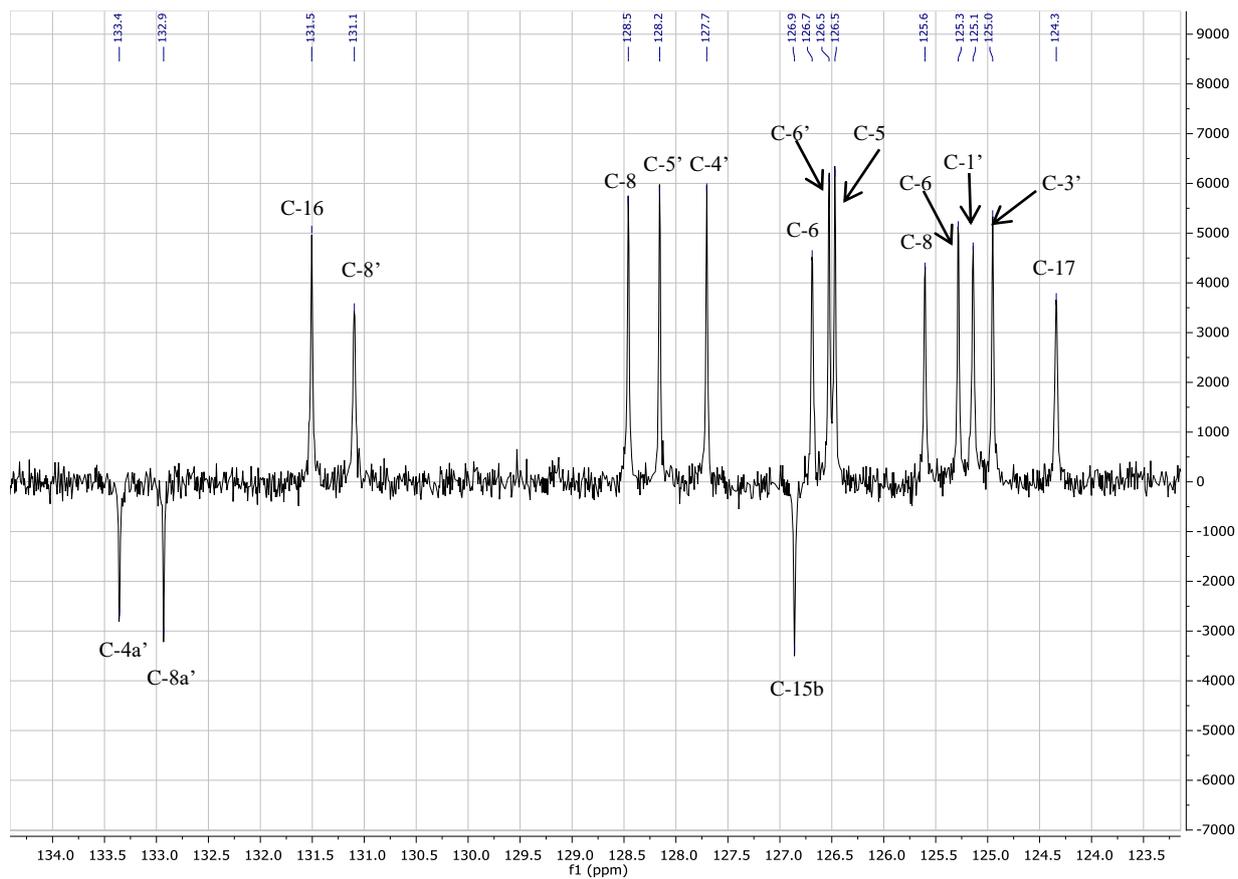
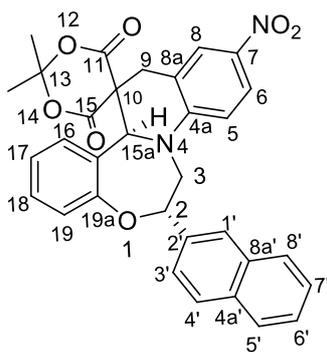


Figure S59. J-modulated ^{13}C -NMR spectrum of *rac*-**11c** measured in CDCl_3 (100 MHz)

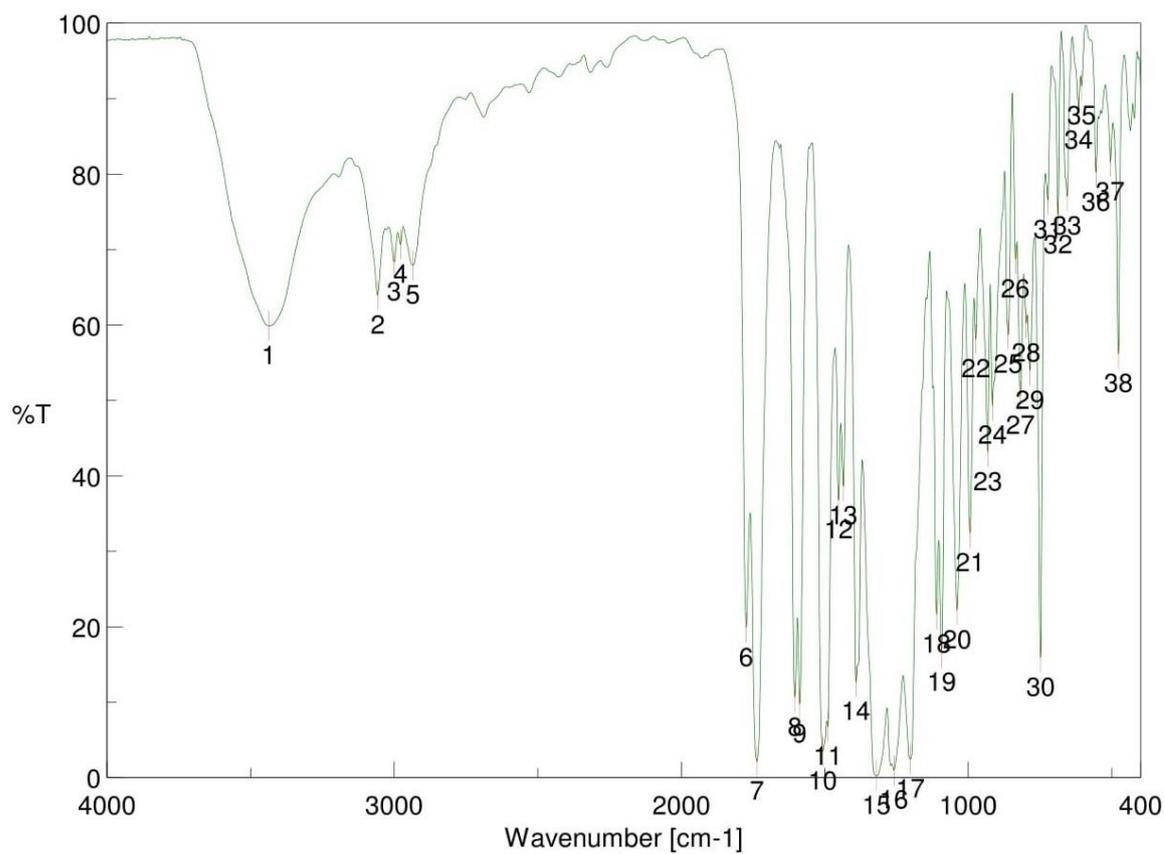
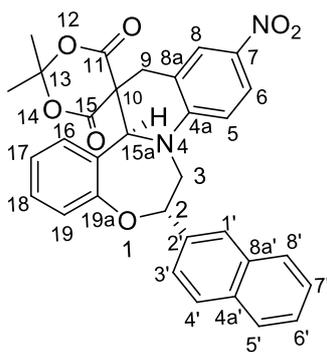


Figure S60. IR spectrum of *rac*-**11c** recorded as KBr disc

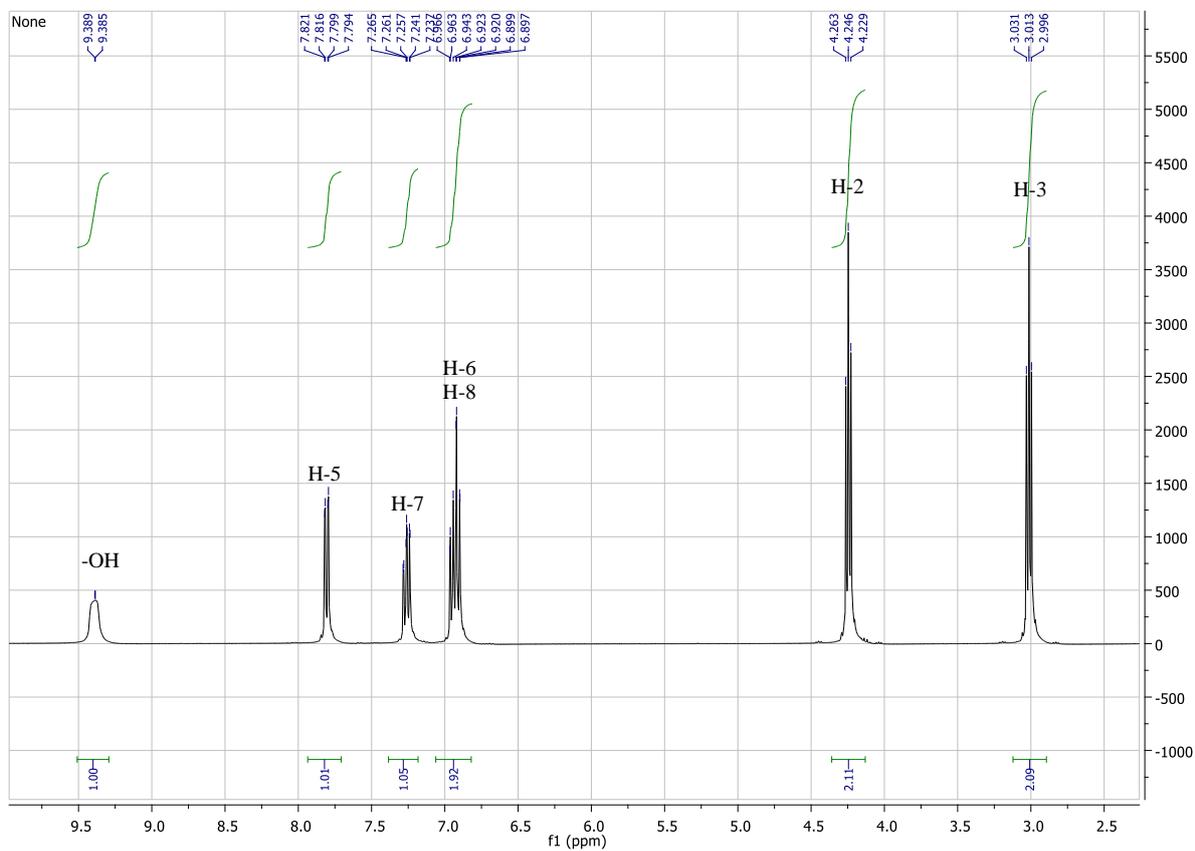
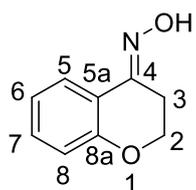


Figure S61. $^1\text{H-NMR}$ spectrum of **13** measured in CDCl_3 (360 MHz)

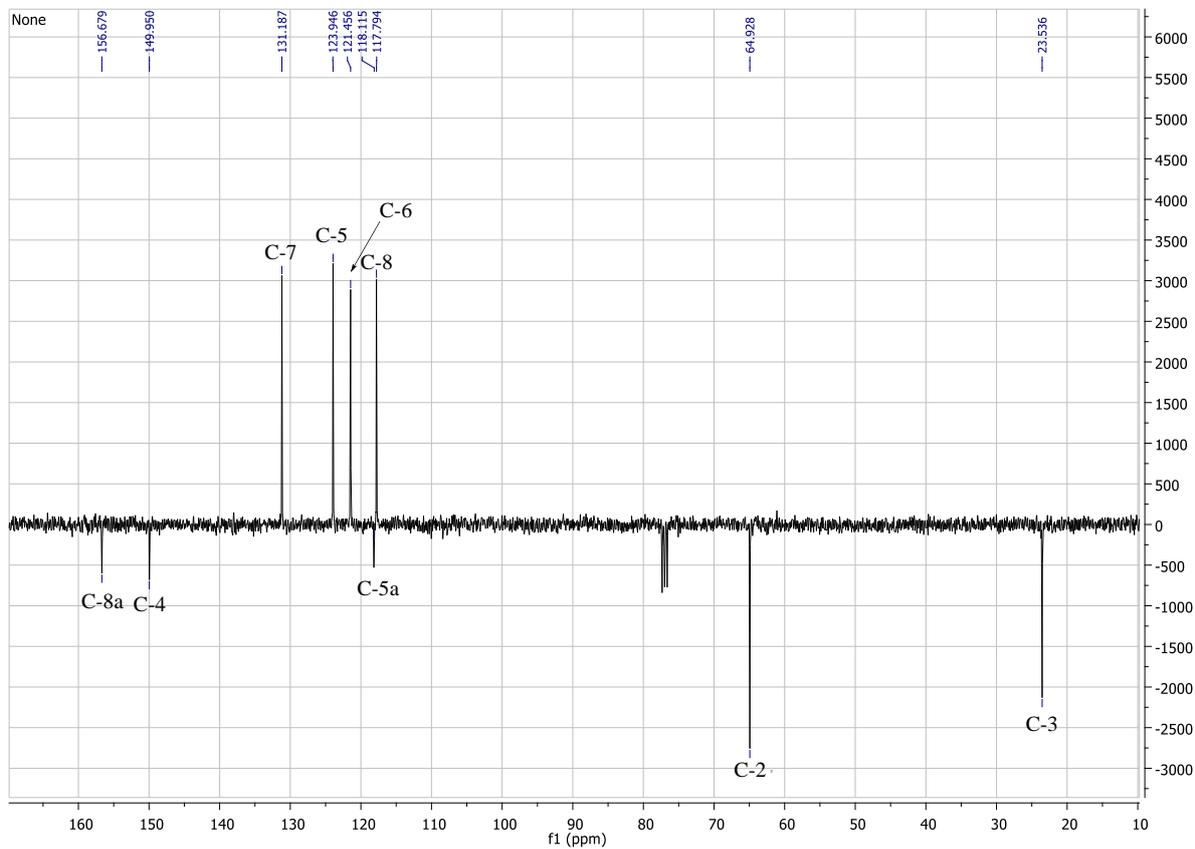
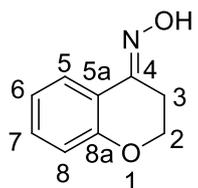


Figure S65. J-modulated ^{13}C -NMR spectrum of **13** measured in CDCl_3 (90 MHz)

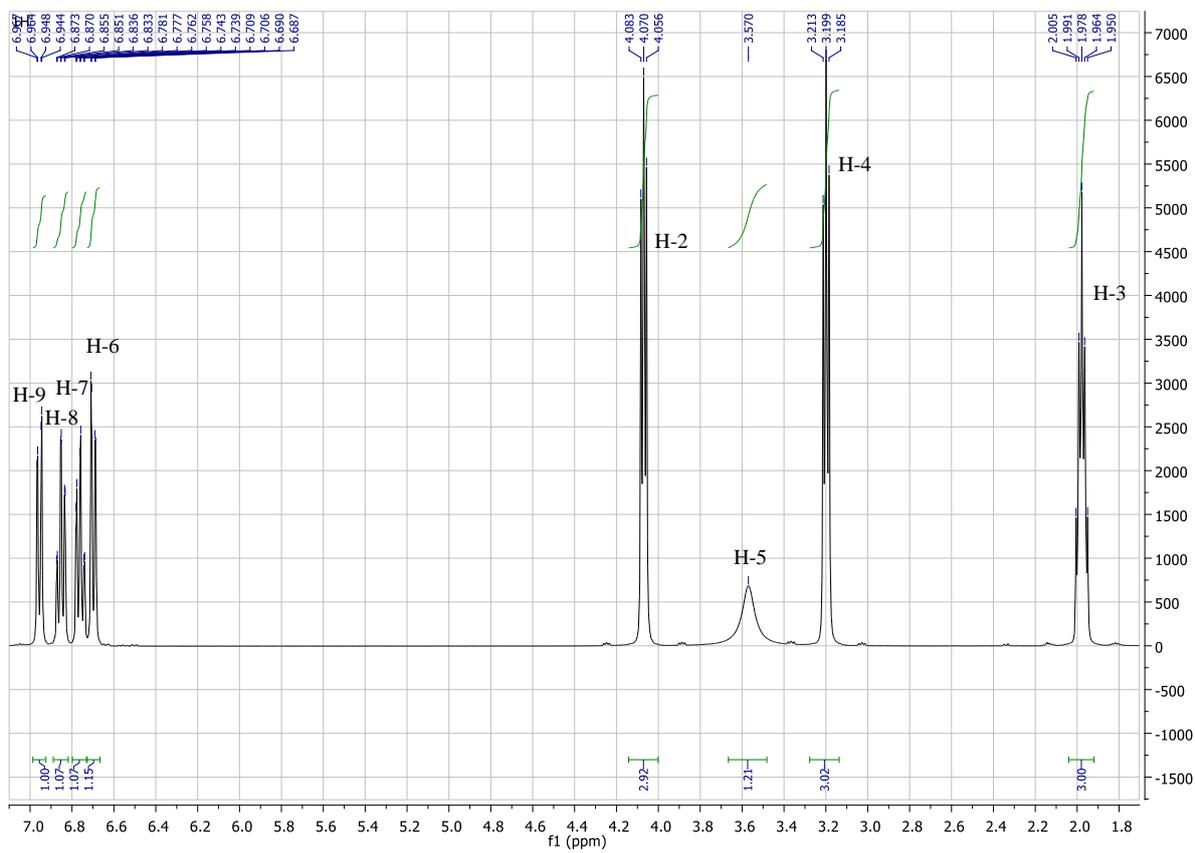
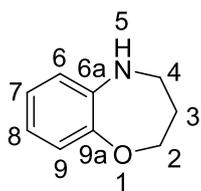


Figure S67. $^1\text{H-NMR}$ spectrum of **15** measured in CDCl_3 (400 MHz)

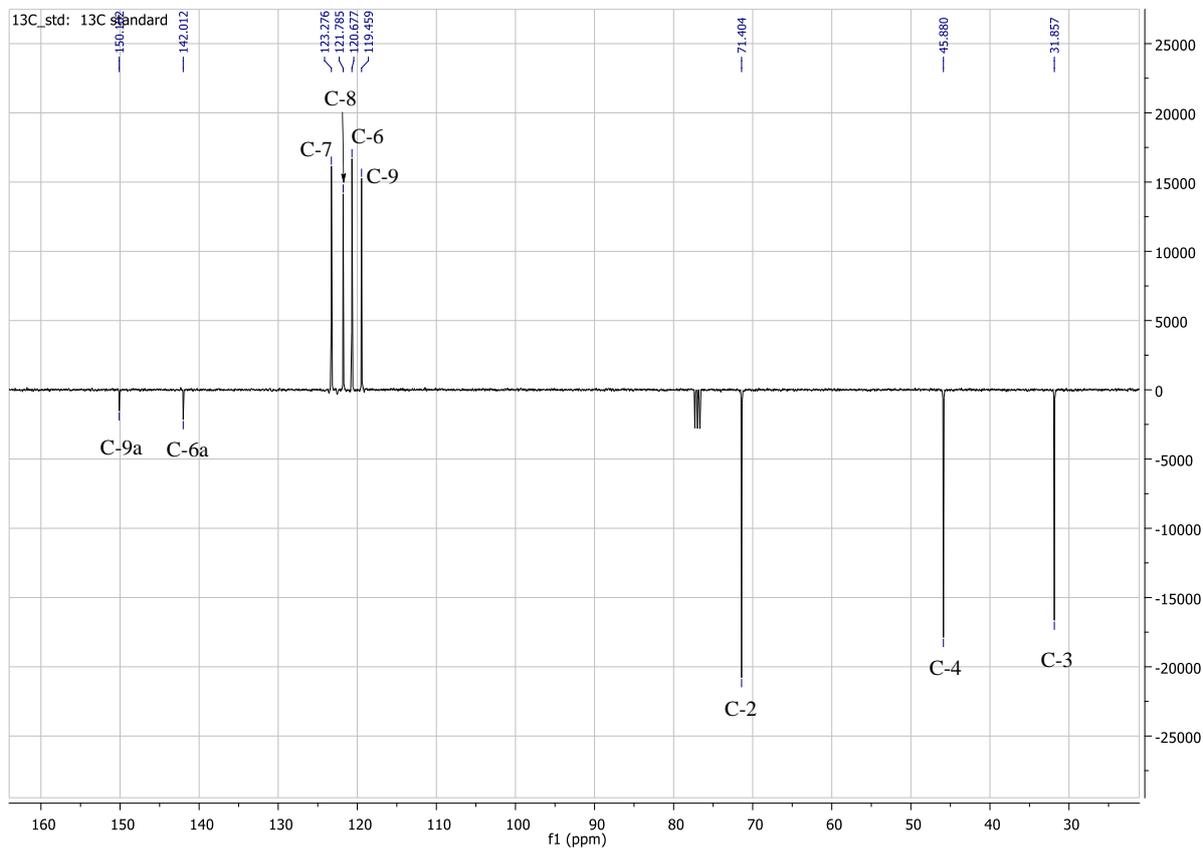
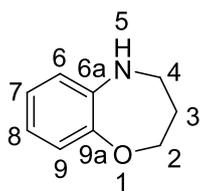


Figure S68. J-modulated ¹³C-NMR spectrum of **15** measured in CDCl₃ (100 MHz)

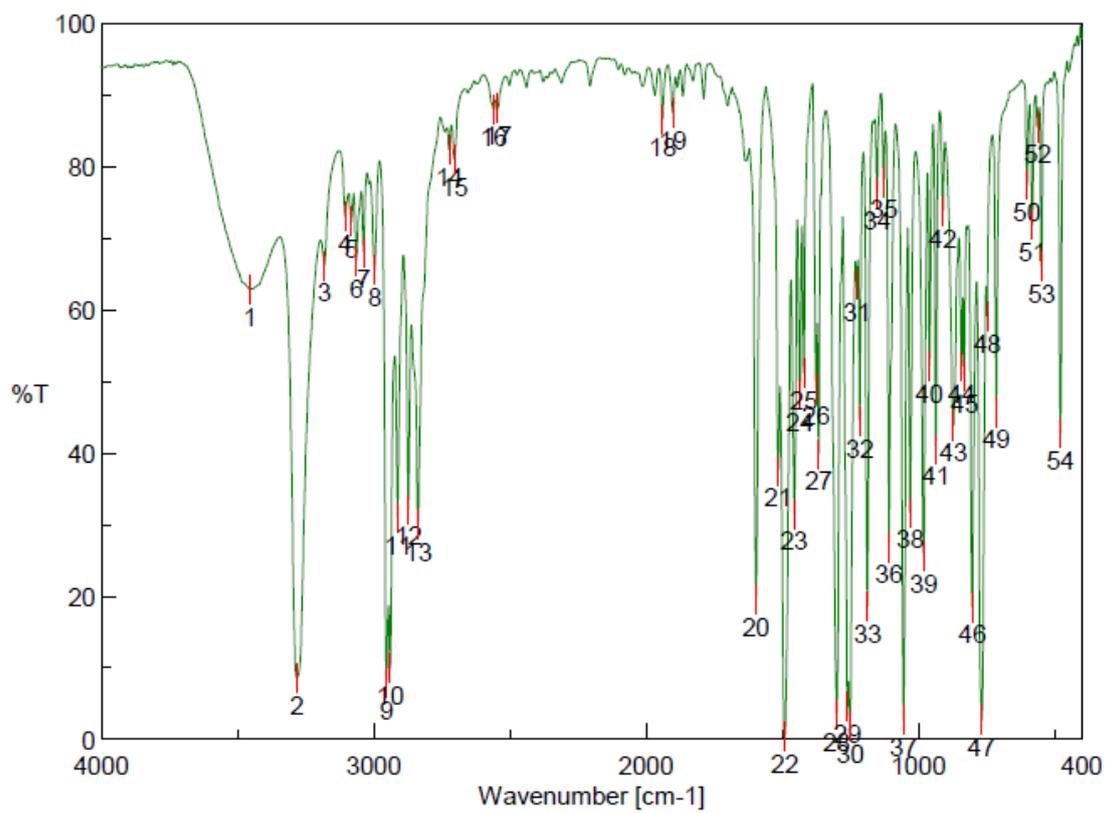
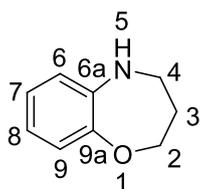


Figure S69. IR spectrum of **15** recorded as KBr disc

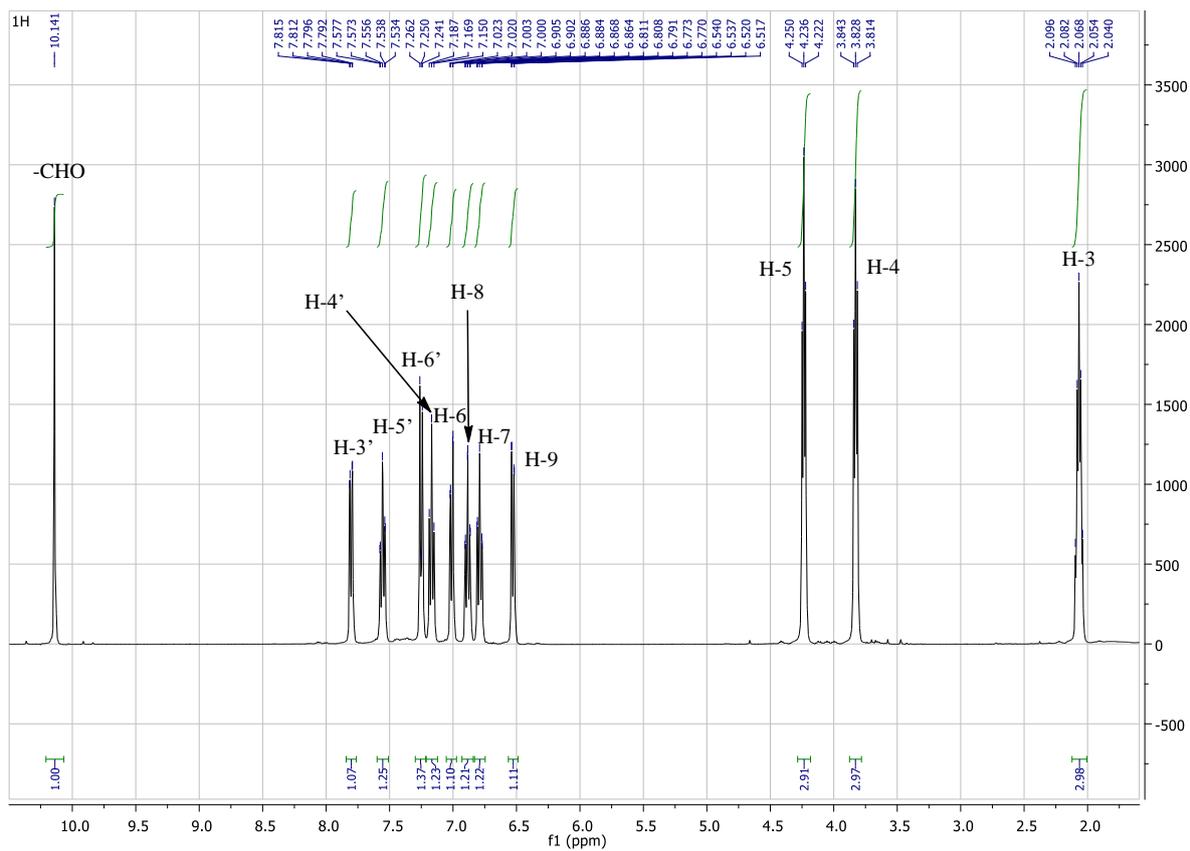
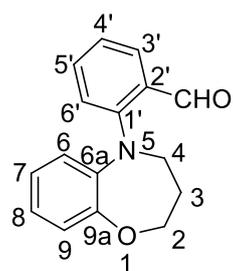


Figure S70. ^1H -NMR spectrum of **4** measured in CDCl_3 (400 MHz)

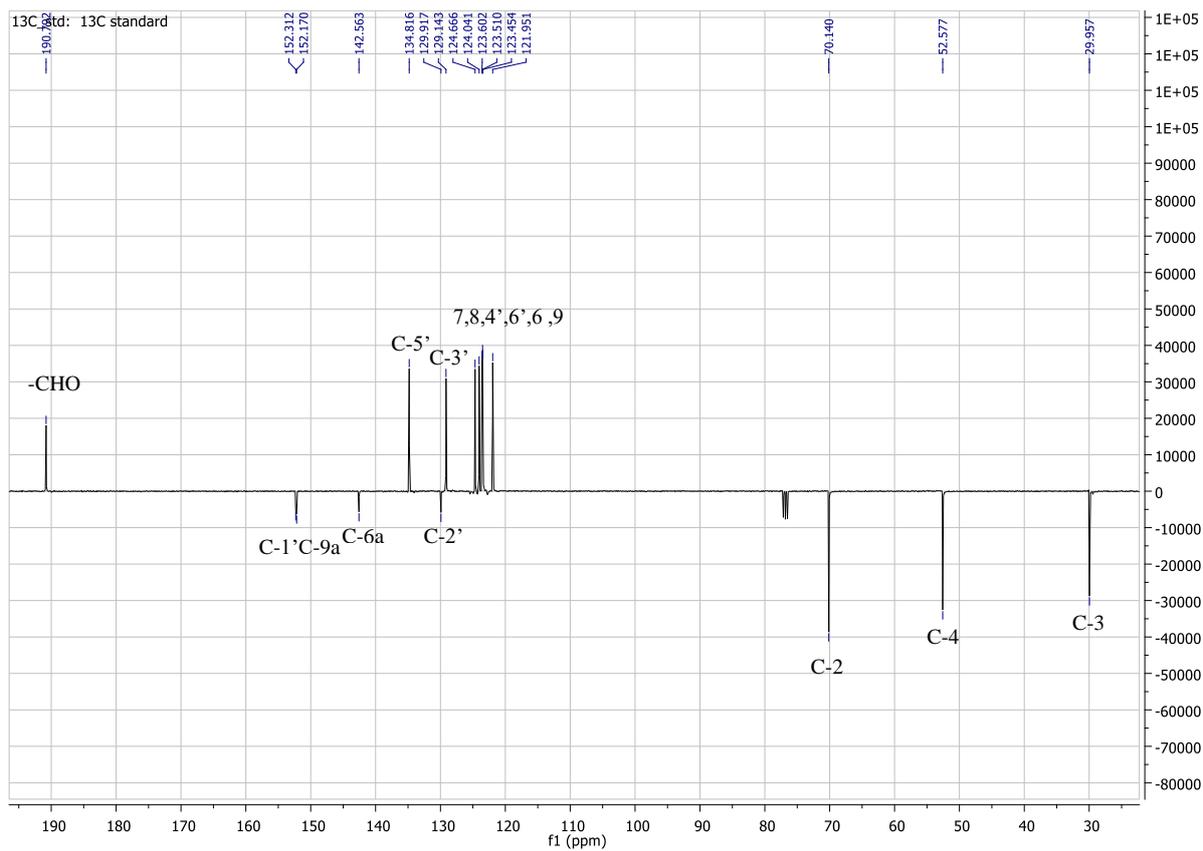
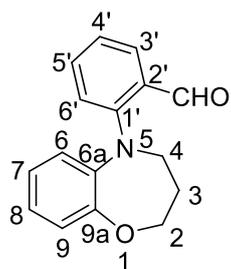


Figure S71. J-modulated ^{13}C -NMR spectrum of **4** measured in CDCl_3 (100 MHz)

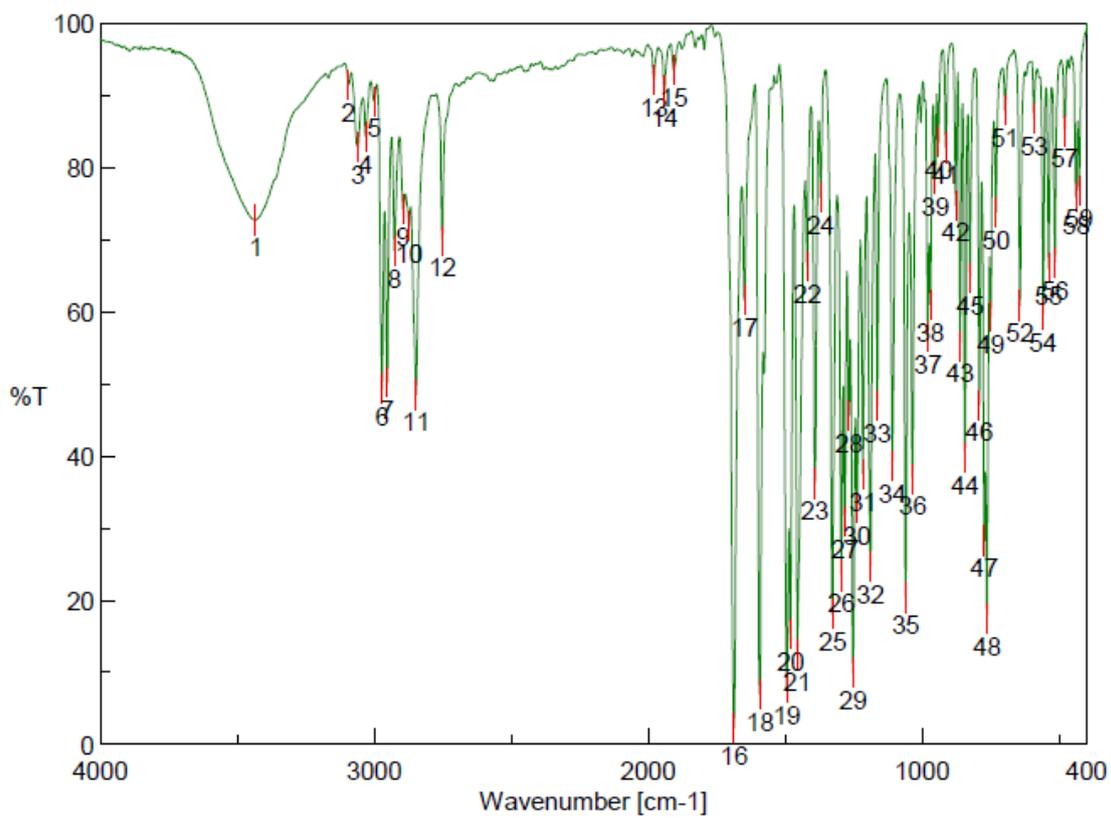
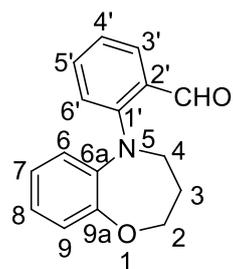


Figure S72. IR spectrum of **4** recorded as KBr disc

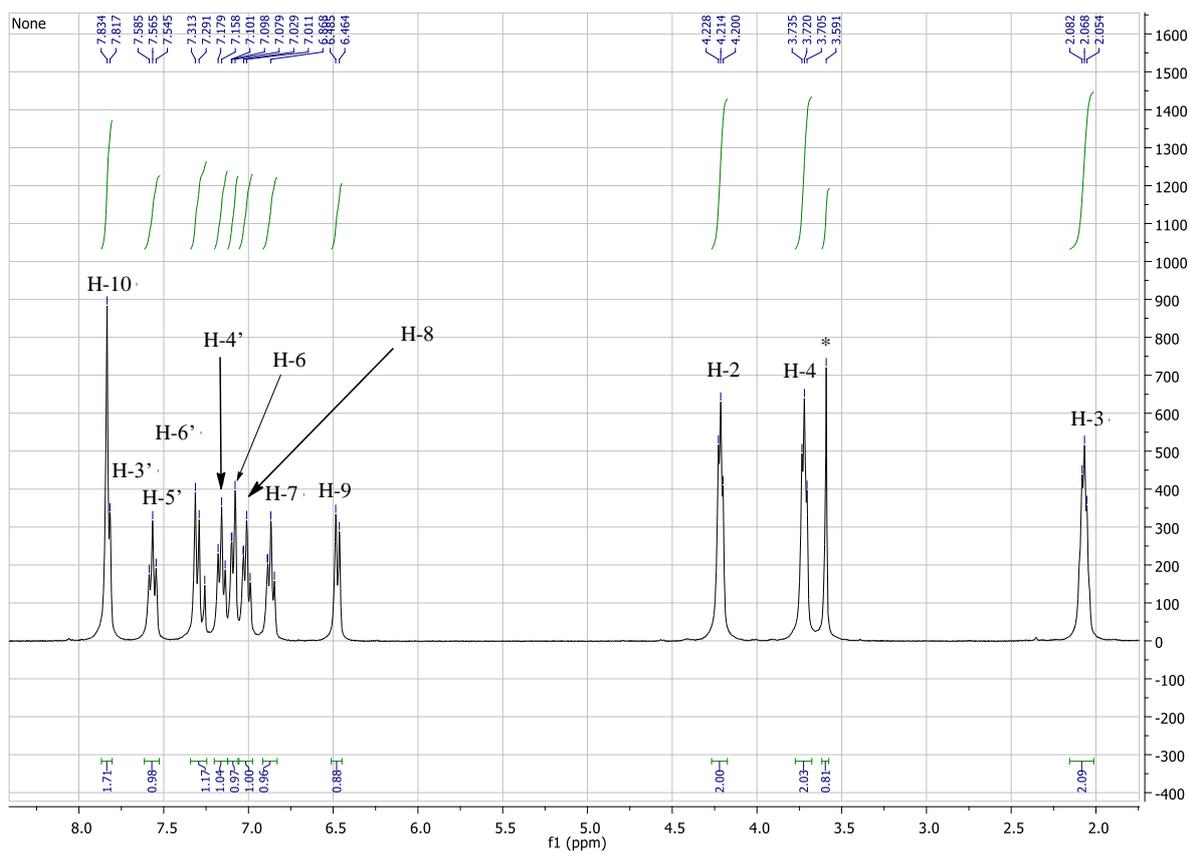
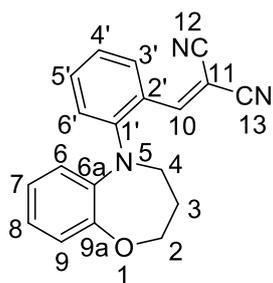


Figure S73. $^1\text{H-NMR}$ spectrum of **20** measured in CDCl_3 (360 MHz)

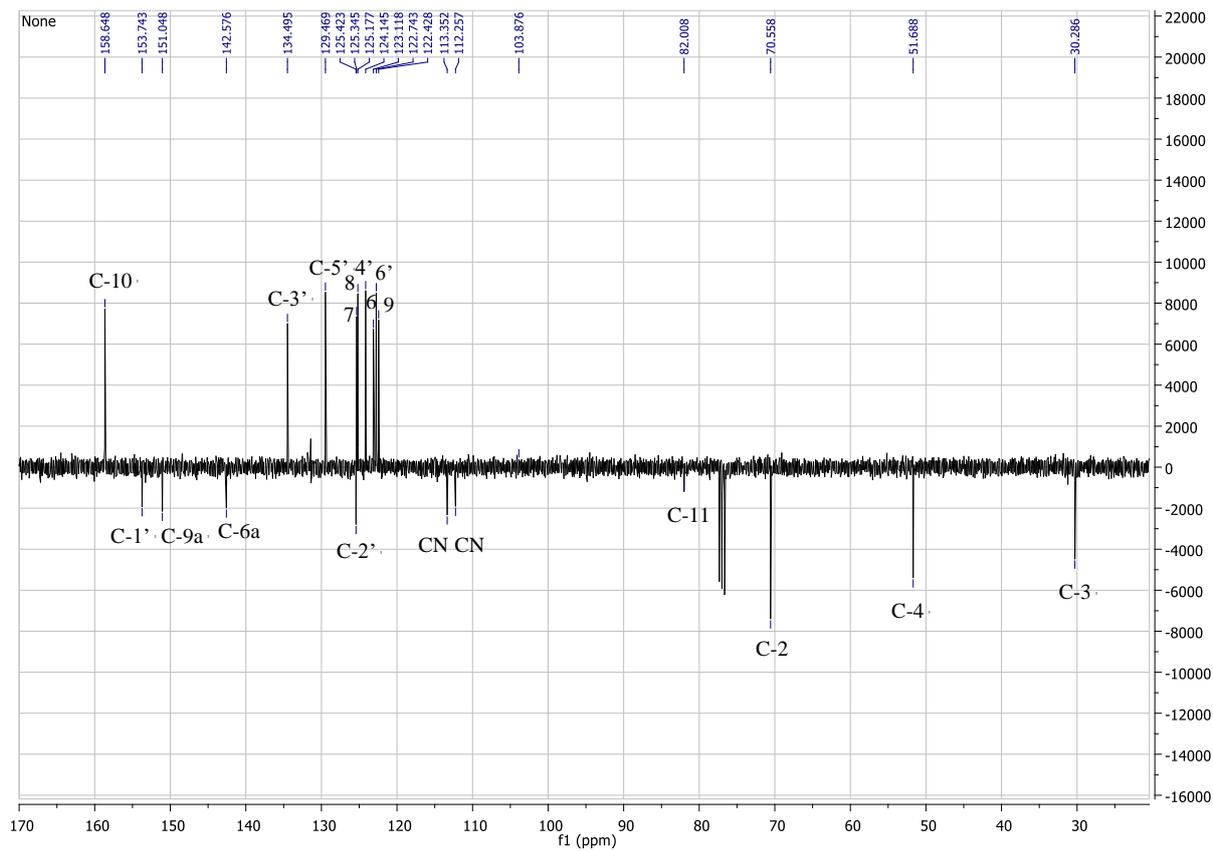
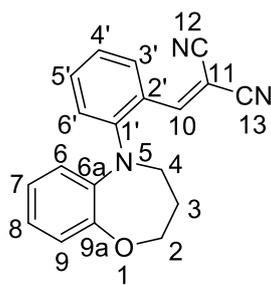


Figure S74. J-modulated ^{13}C -NMR spectrum of **20** measured in CDCl_3 (90 MHz)

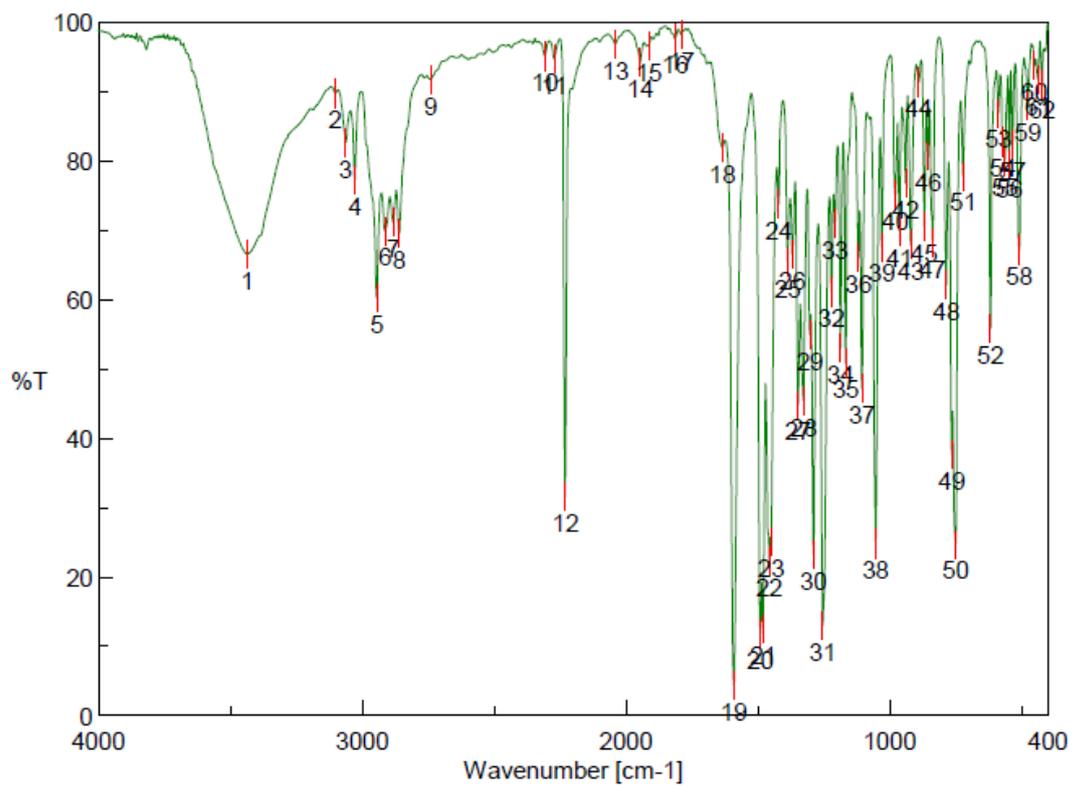
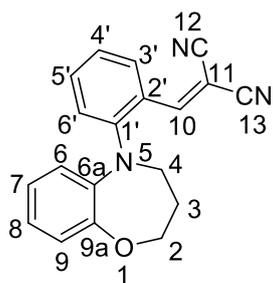


Figure S75. IR spectrum of **20** recorded as KBr disc

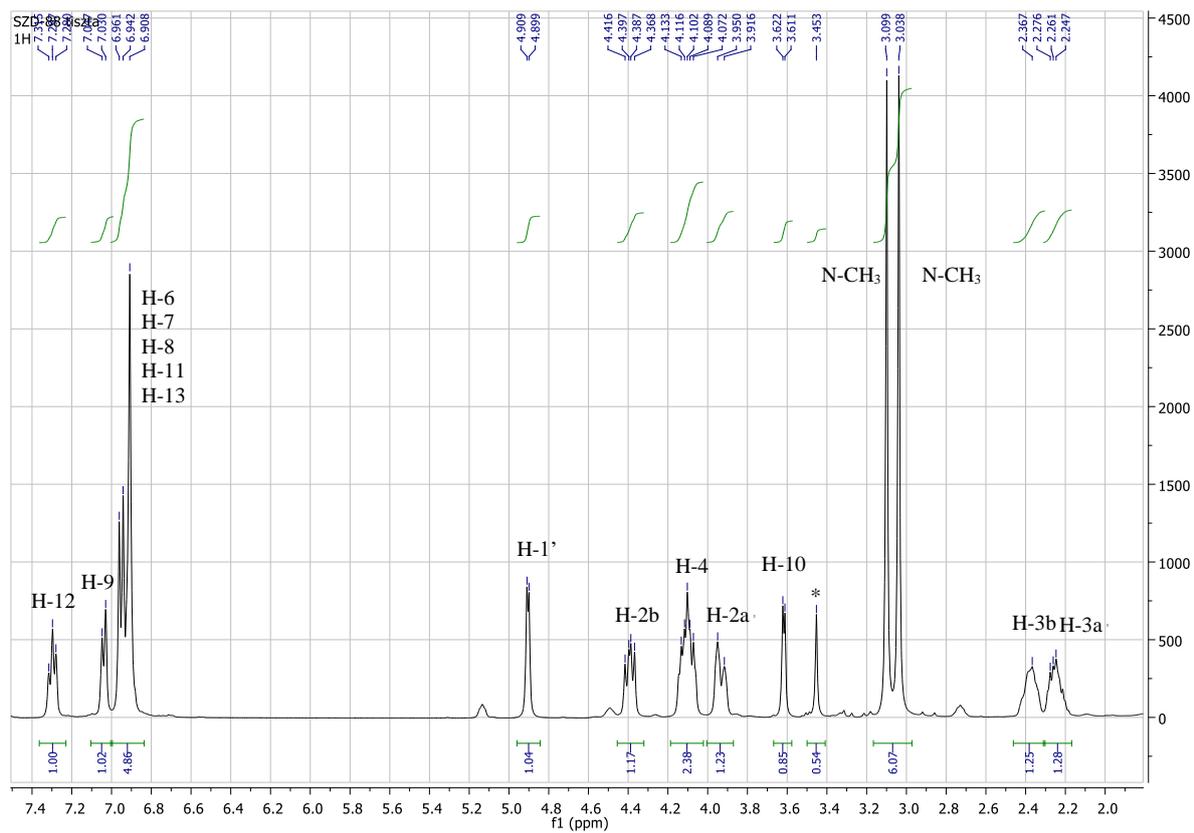
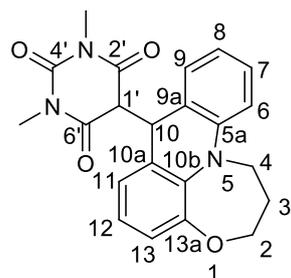


Figure S76. $^1\text{H-NMR}$ spectrum of **6** measured in CDCl_3 (400 MHz)

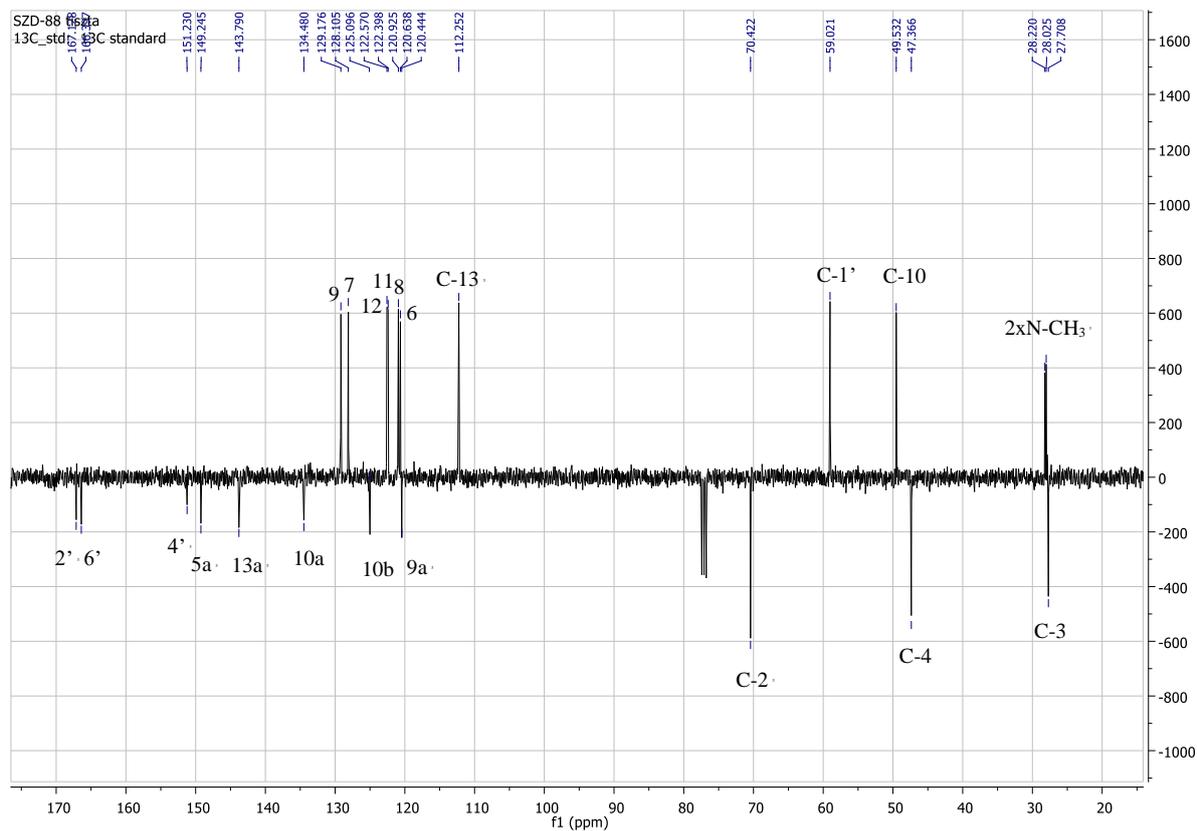
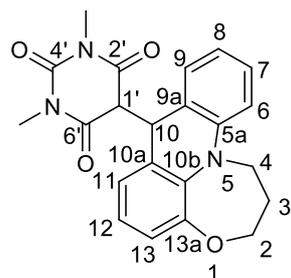


Figure S77. J-modulated ^{13}C -NMR spectrum of **6** measured in CDCl_3 (100 MHz)

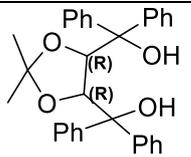
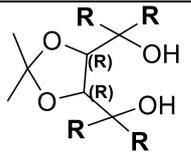
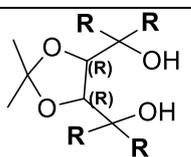
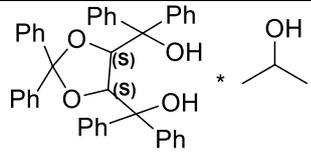
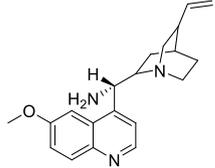
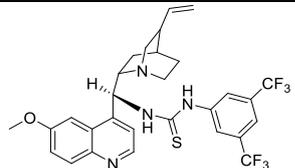
organocatalyst	Reaction time (day)		Conversion (%)		ee (%)	
	A	B	A	B	A	B
	21	9	22	25	6.1	6.9
 R: α -naphthyl	21	9	26	26	7.3	5.4
 R: β -naphthyl	21	9	17	29	7.2	3.8
	21	9	13	30	4.6	2.9
	8	8	10	11	2.9	1.9
	8	8	9	8	0.0	1.0

Table S1. Organocatalytic transformations of **1a** to *trans*-**10a** (columns A) and **1a** to **11a** (columns B); reaction condition: MgSO₄/CHCl₃, 0.3 equivalent of organocatalyst, rt.

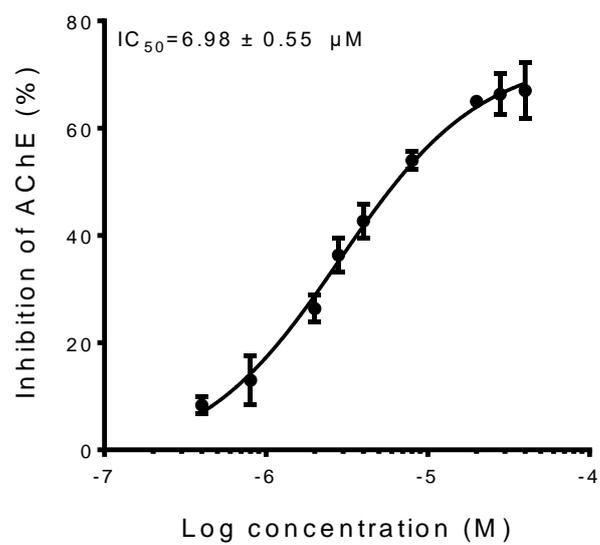


Figure S78. Concentration-dependent curve of **6** for the inhibition of AChE activity. IC_{50} of **6** was calculated to be $6.98 \pm 0.55 \mu M$. Every point is an average of three independent experiments (mean \pm SD).