

From Nitrobenzenes to Substituted Tetrahydroquinolines in a Single Step by a Domino Reduction / Imine Formation / Aza-Diels–Alder Reaction

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Supporting Information

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(3a*SR*,4*RS*,9b*RS*)-4-Phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5a**)

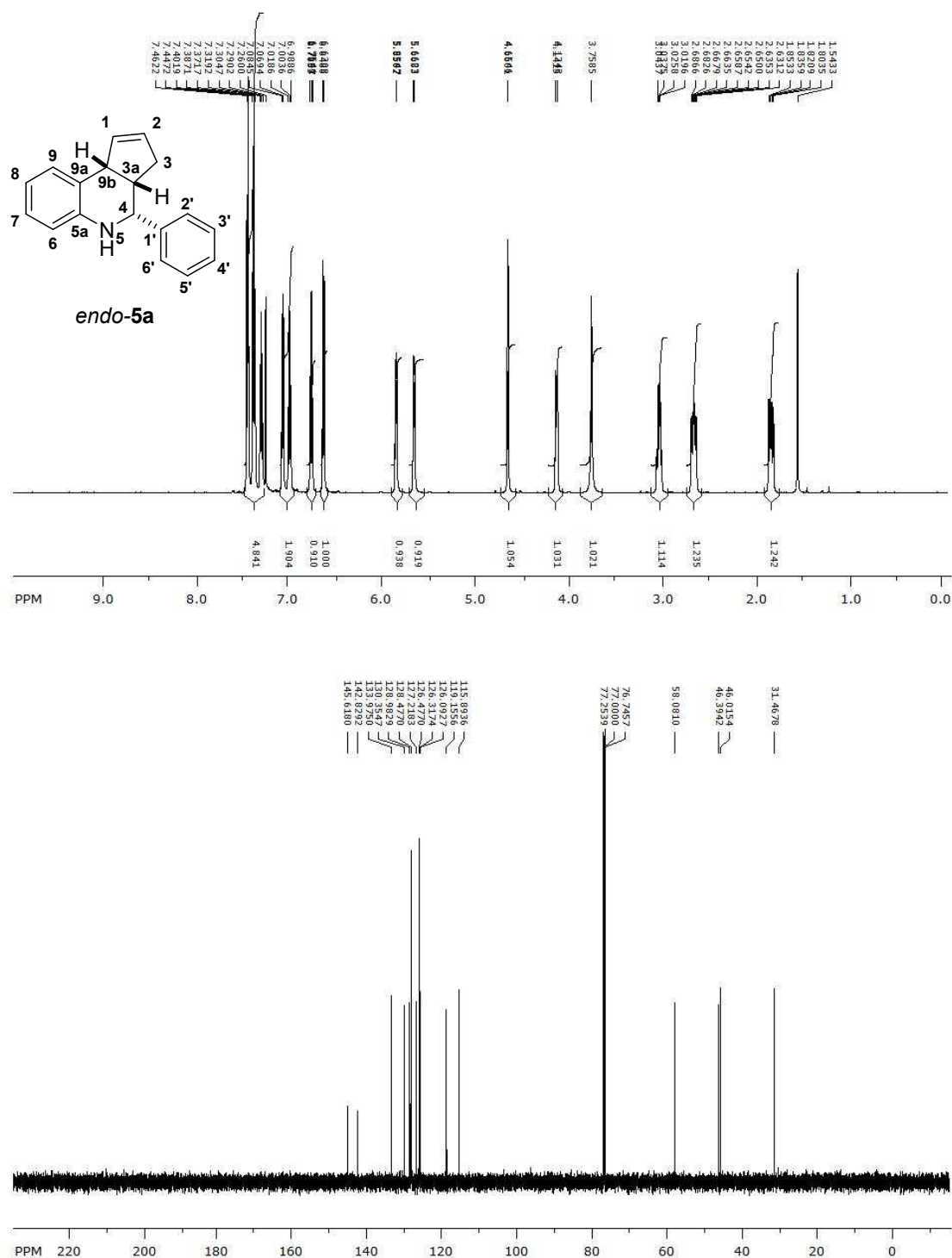
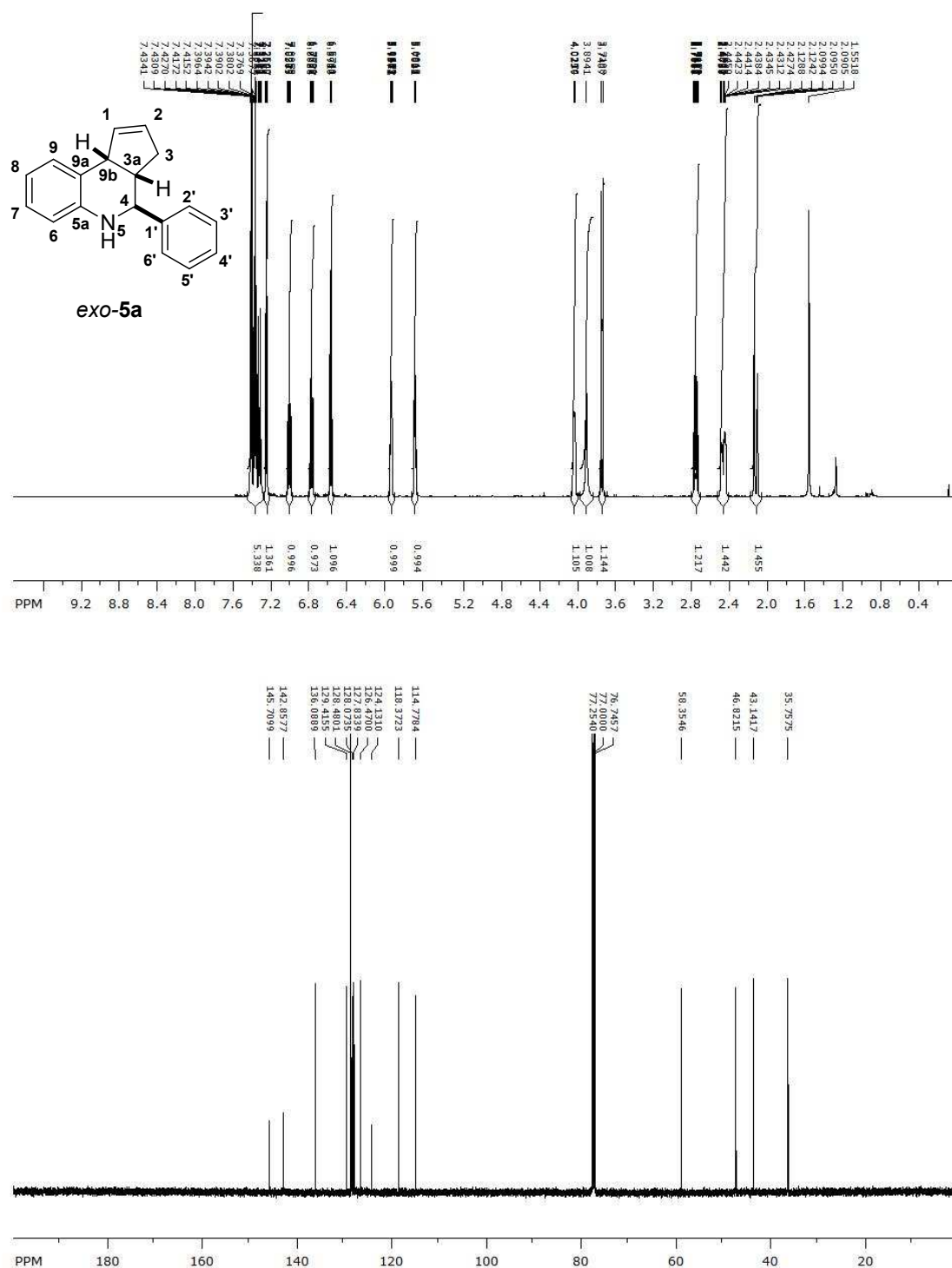


Figure 1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra of *endo*-**5a** in CDCl_3 .

(3a*SR*,4*SR*,9b*RS*)-4-Phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*exo*-**5a**)



(3aSR,4RS,9bRS)-6-Bromo-4-phenyl-3a,4,5,9b-tetrahydro-3H-cyclopenta[*c*]quinoline (*endo*-5b)

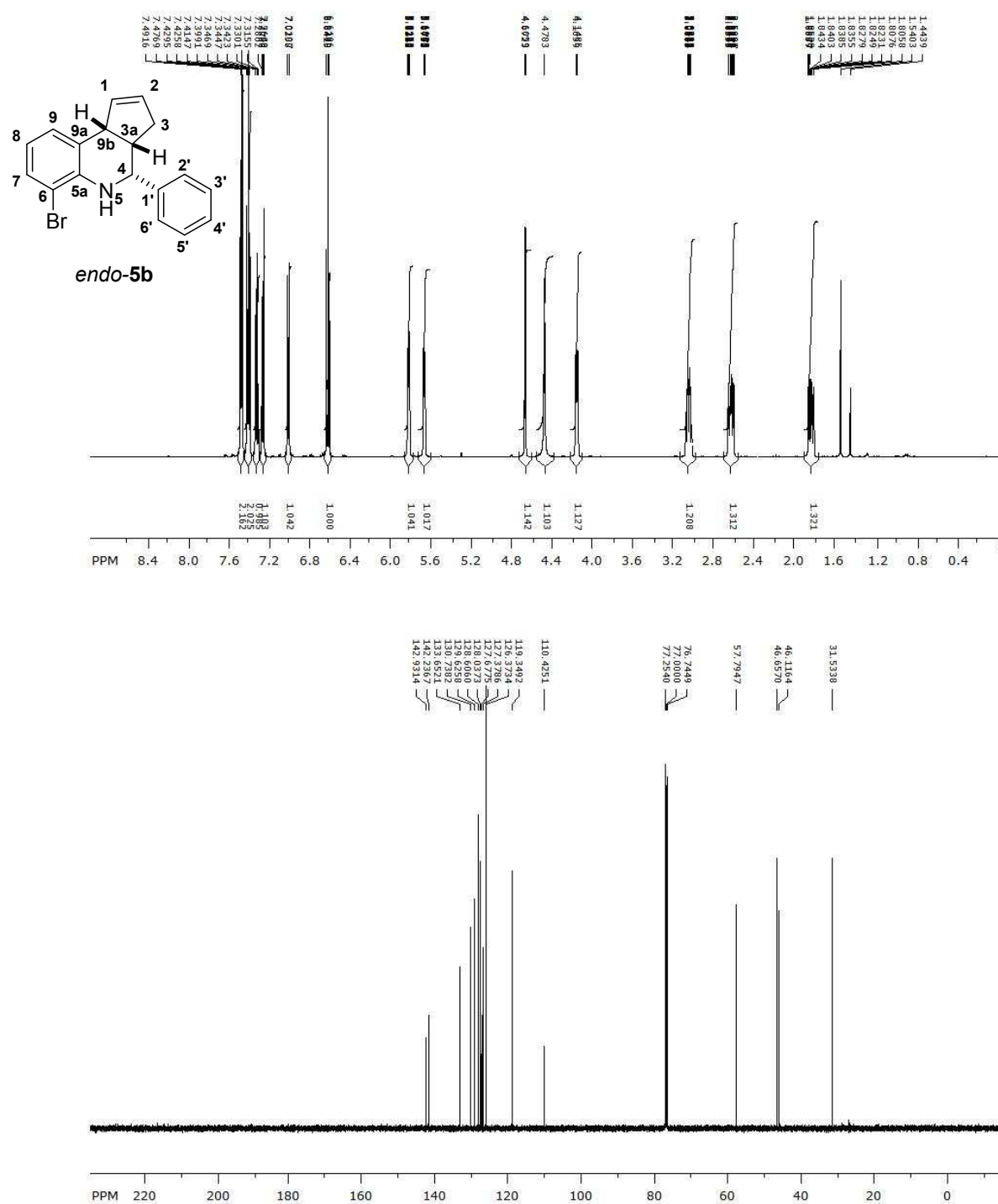


Figure 3. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra of *endo*-**5b** in CDCl_3 .

(3a*SR*,4*RS*,9b*RS*)-7-Bromo-4-phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5c**)

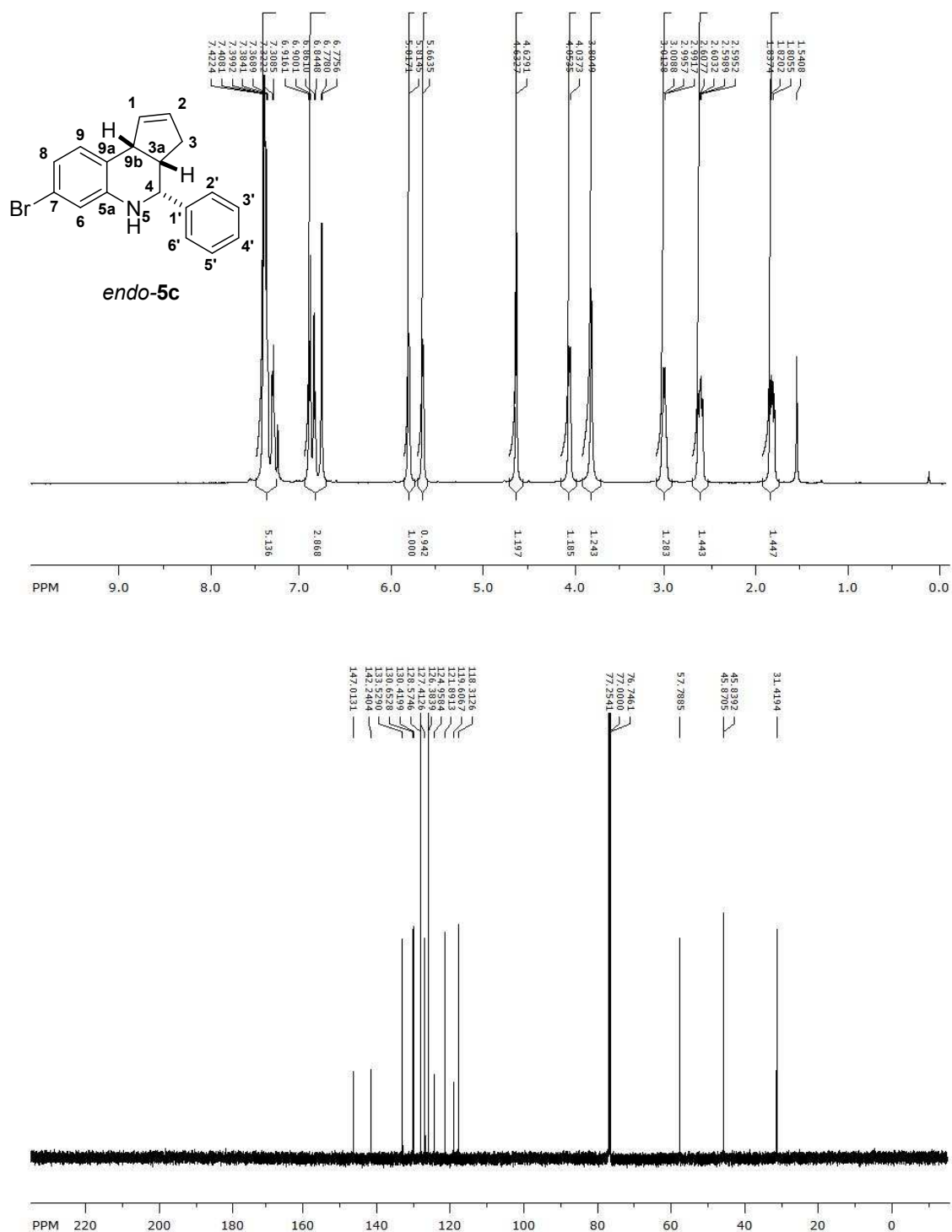


Figure 4. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-**5c** in CDCl₃.

***endo*-5d**

¹H NMR (400 MHz, CDCl₃):

Chemical Shift (ppm)	Integration
7.4360, 7.4332, 7.4189, 7.3996, 7.3955, 7.3848, 7.3228, 7.3200	3.794
7.2868, 7.2808, 7.1770, 7.0486	0.845
6.8932	0.832
5.6072, 5.6028	0.905
5.0288	0.927
4.6048	1.025
4.0278	1.025
3.7801	0.969
2.6110, 2.6088, 2.5922, 2.5876	1.081
2.154	1.154
1.8525, 1.8490, 1.8320, 1.8304, 1.8152, 1.7978, 1.7945	1.157

¹³C NMR (100 MHz, CDCl₃):

Chemical Shift (ppm)	
144.6512, 143.9812, 133.4015, 131.5285, 130.8635, 129.0326, 128.2029, 127.3729, 126.3935, 117.4149, 110.6510	
76.7460, 77.0000, 77.2536	
57.9321	
46.2113, 45.7236	
31.4029	

S6

(3a*SR*,4*SR*,9b*RS*)-8-Bromo-4-phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*exo*-5d)

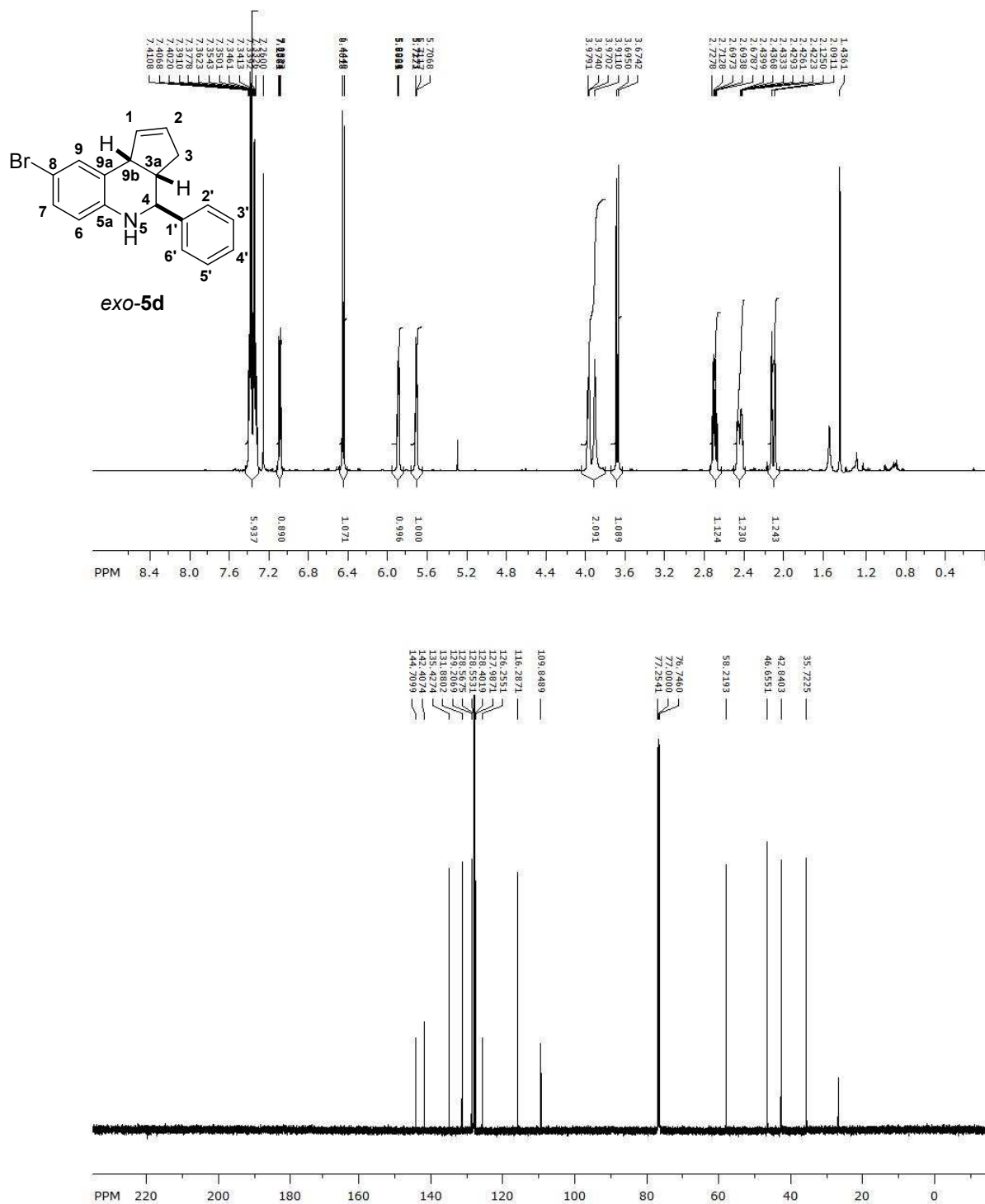


Figure 6. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *exo*-5d in CDCl₃.

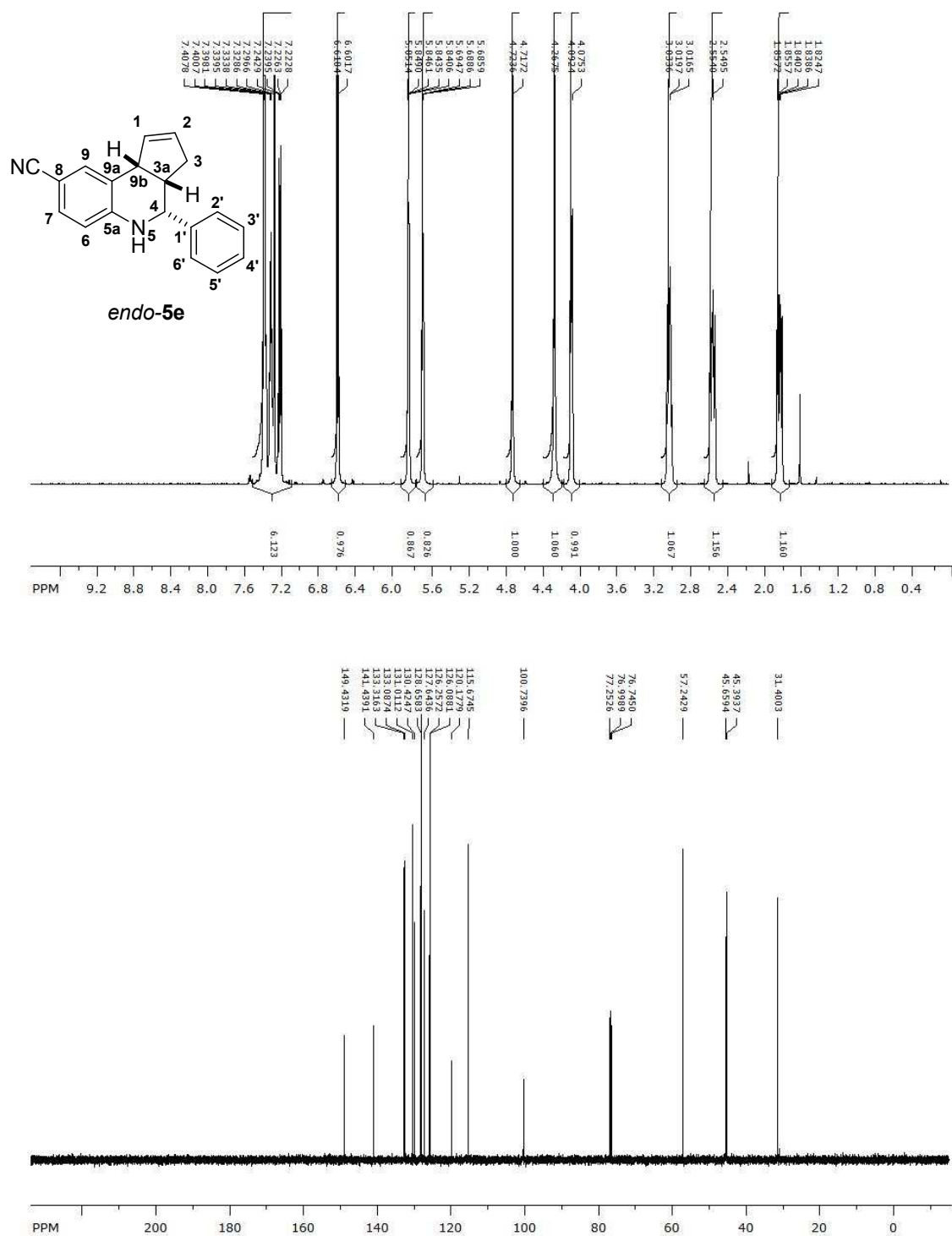


Figure 7. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra of *endo-5e* in CDCl_3 .

(3a*SR*,4*RS*,9b*RS*)-8-Methoxy-4-phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline
(*endo*-**5f**)

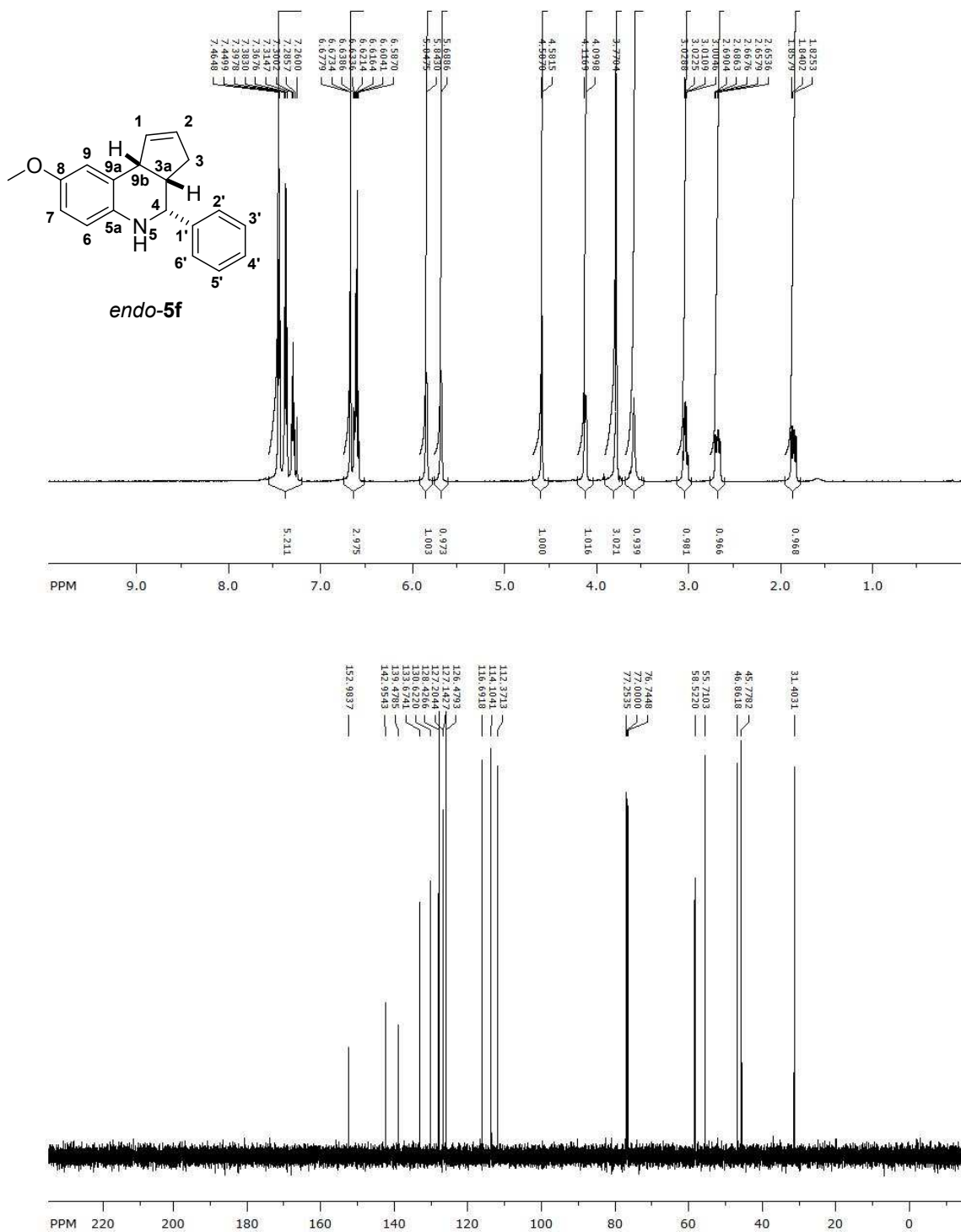


Figure 8. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-**5f** in CDCl₃.

Chemical structure of endo-5g:

C[C@H]1C[C@@H]2[C@H]3C=C[C@H]3[C@@H]2[C@H]1c1ccc(N)cc1

¹H NMR (400 MHz, CDCl₃) data:

Chemical Shift (ppm)	Integration
7.4650, 7.4550, 7.4450, 7.4350, 7.3839, 7.3684, 7.3450, 7.3150, 7.2600	0.793, 1.886
6.8277, 6.8223, 6.8173, 6.5563, 5.8642, 5.8589, 5.8473, 5.6664, 5.6604, 5.0786, 5.0733	0.920, 0.895, 0.862, 0.827
4.6446, 4.6207	1.002
4.1035, 4.0861	1.005
3.4492	1.060
3.0254, 3.0189, 3.0124	1.102
2.6566, 2.6513, 2.6329, 2.6324	1.215
2.2619, 2.2510, 2.2379	3.125
1.8310, 1.8337, 1.8377, 1.8010, 1.8153, 1.8243, 1.8301	1.222
1.7978	

¹³C NMR (100 MHz, CDCl₃) data:

Chemical Shift (ppm)
143.1426, 143.0900, 142.8471, 139.3864, 129.3609, 128.4371, 127.0012, 127.1547, 126.4938, 115.8980, 115.8282, 77.2541, 77.0000, 76.7459, 58.2842, 46.4367, 46.0146, 31.3879, 20.5805

S10

(3a*SR*,4*RS*,9b*RS*)-4-(4-Chlorophenyl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5i**)

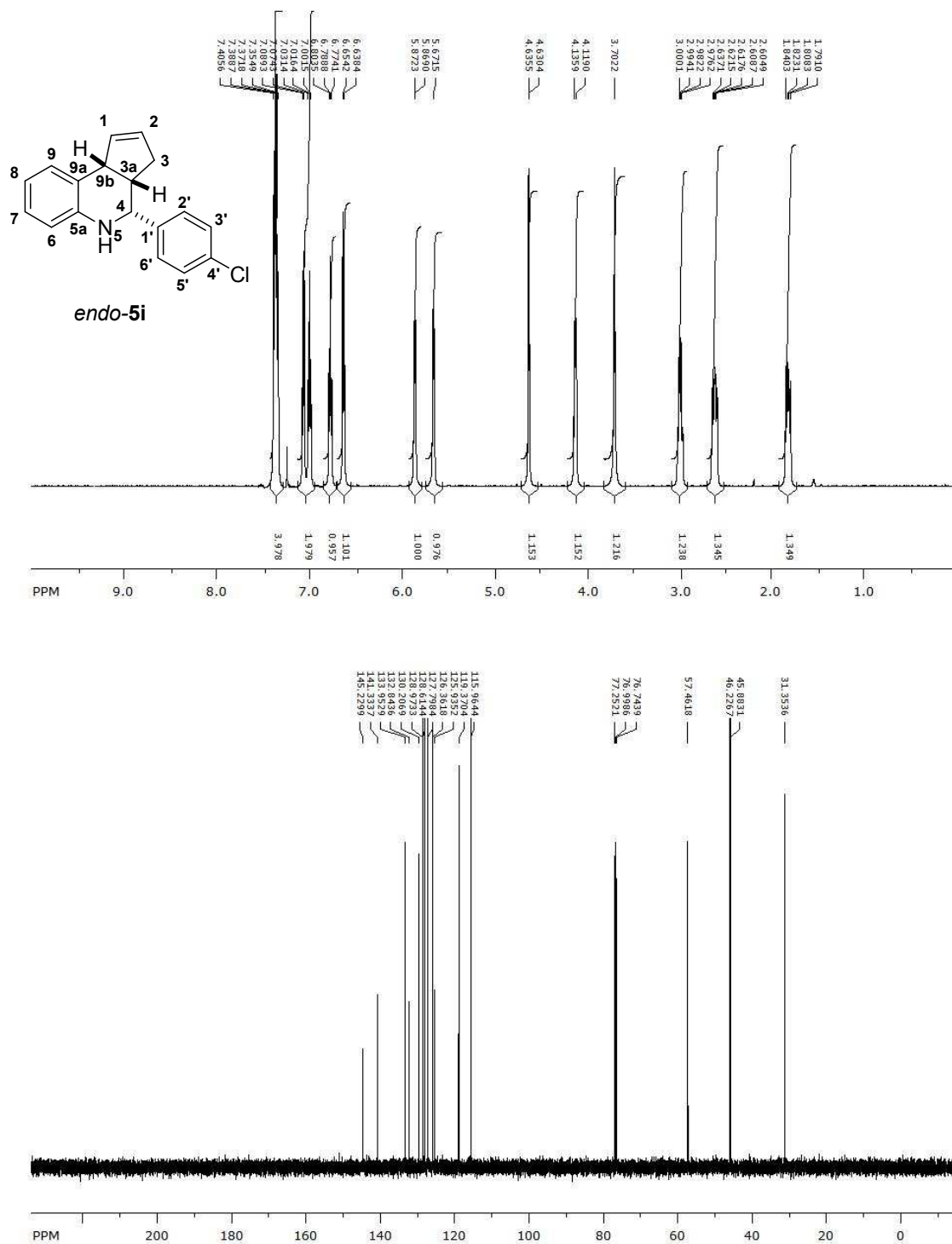


Figure 11. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-**5i** in CDCl₃.

(3a*SR*,4*RS*,9b*RS*)-4-(4-Bromophenyl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5j**)

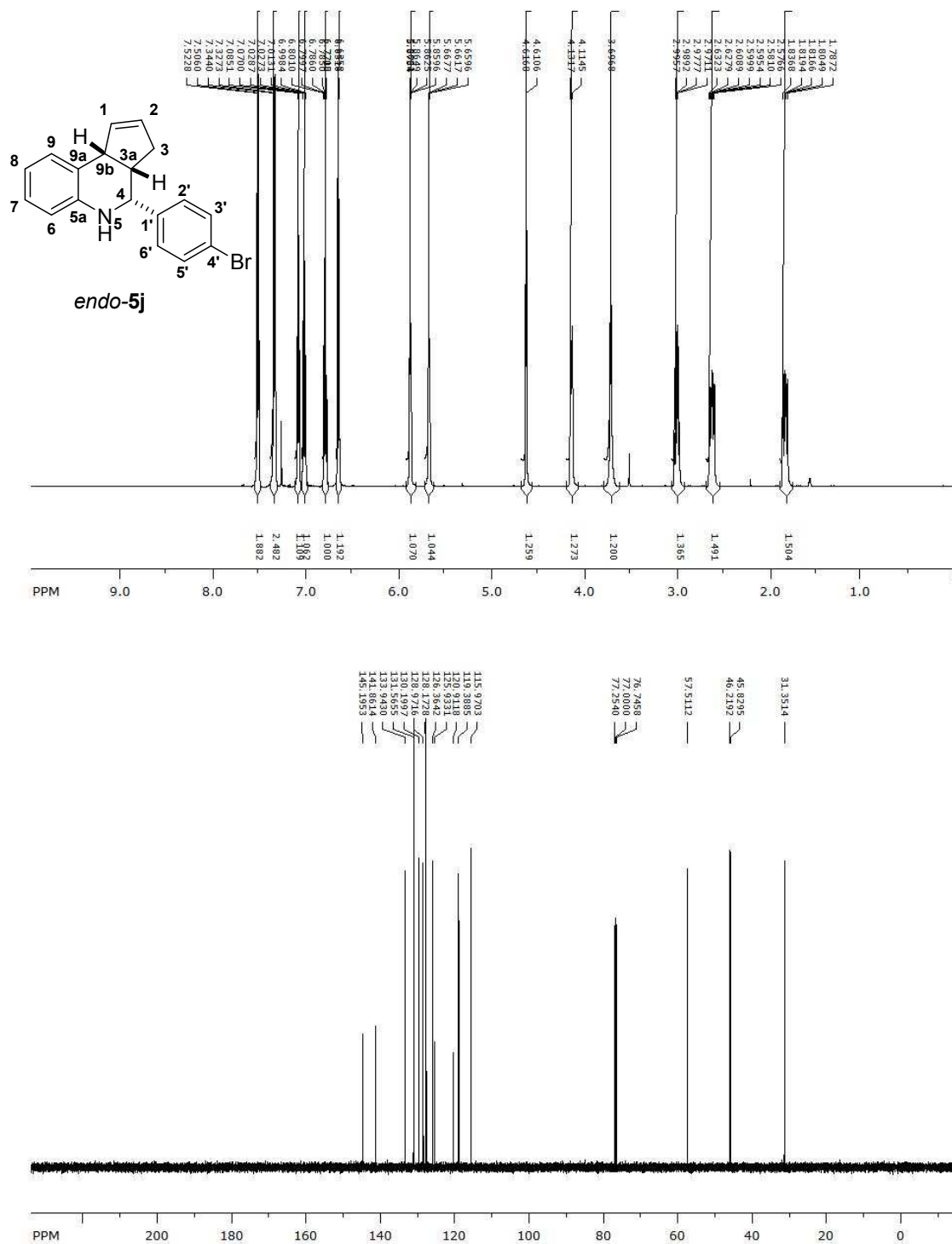


Figure 12. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-**5j** in CDCl₃.

4-((3a*SR*,4*RS*,9b*RS*)-3a,4,5,9b-Tetrahydro-3*H*-cyclopenta[*c*]quinolin-4-yl)benzonitrile (*endo*-5k)

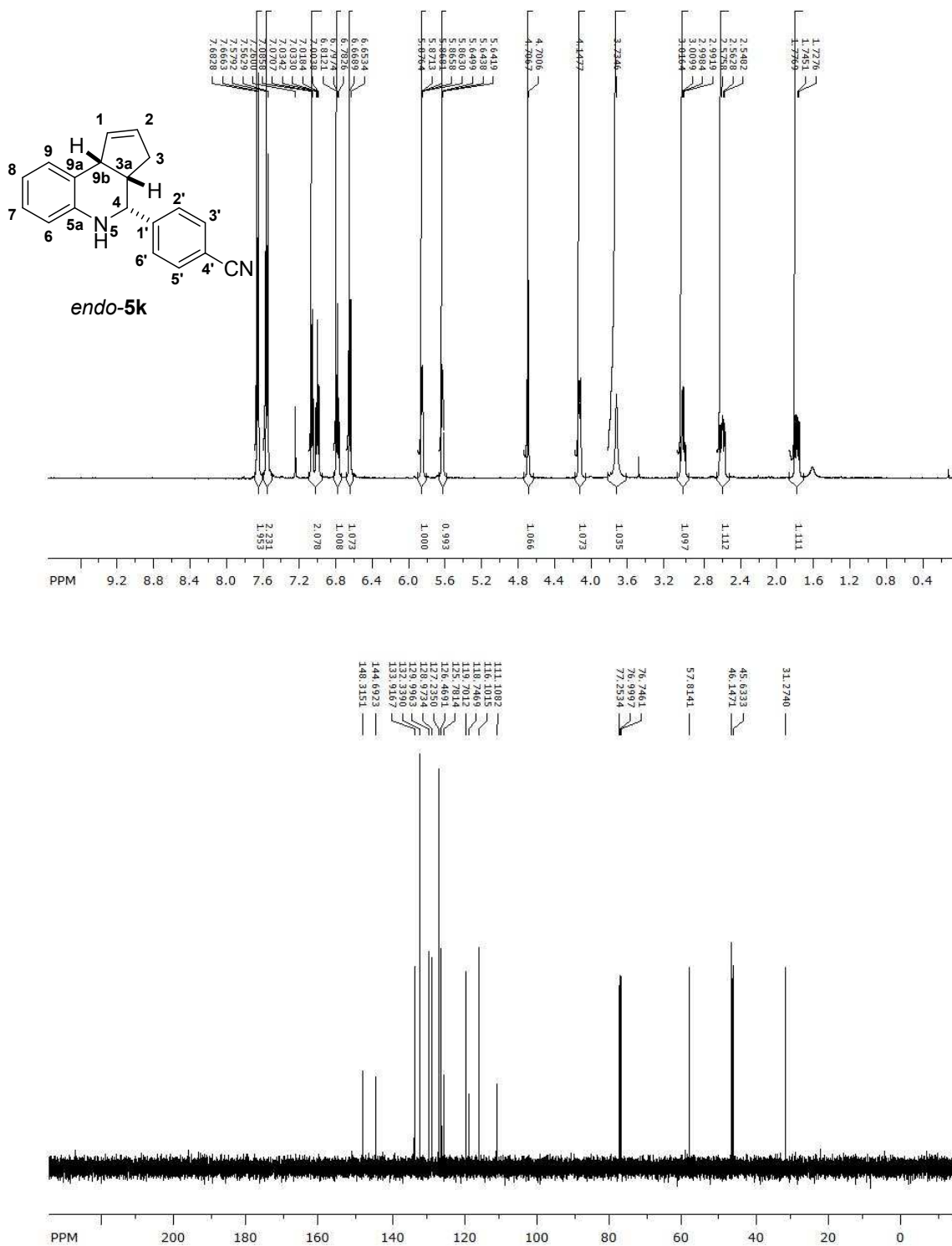


Figure 13. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-5k in CDCl₃.

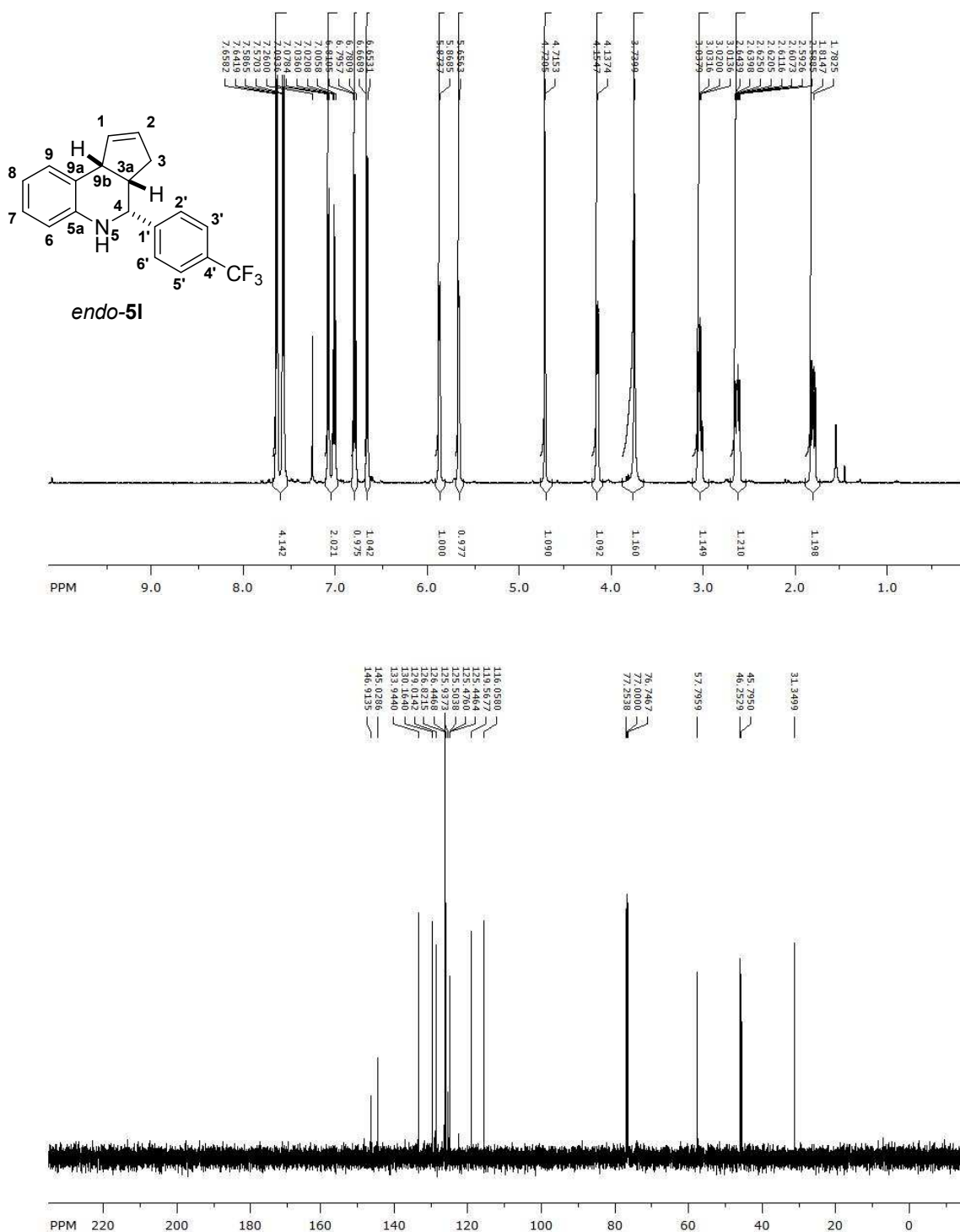


Figure 14. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra of *endo*-**5l** in CDCl_3 .

(3a*SR*,4*RS*,9b*RS*)-4-(Methoxyphenyl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-5*m*)

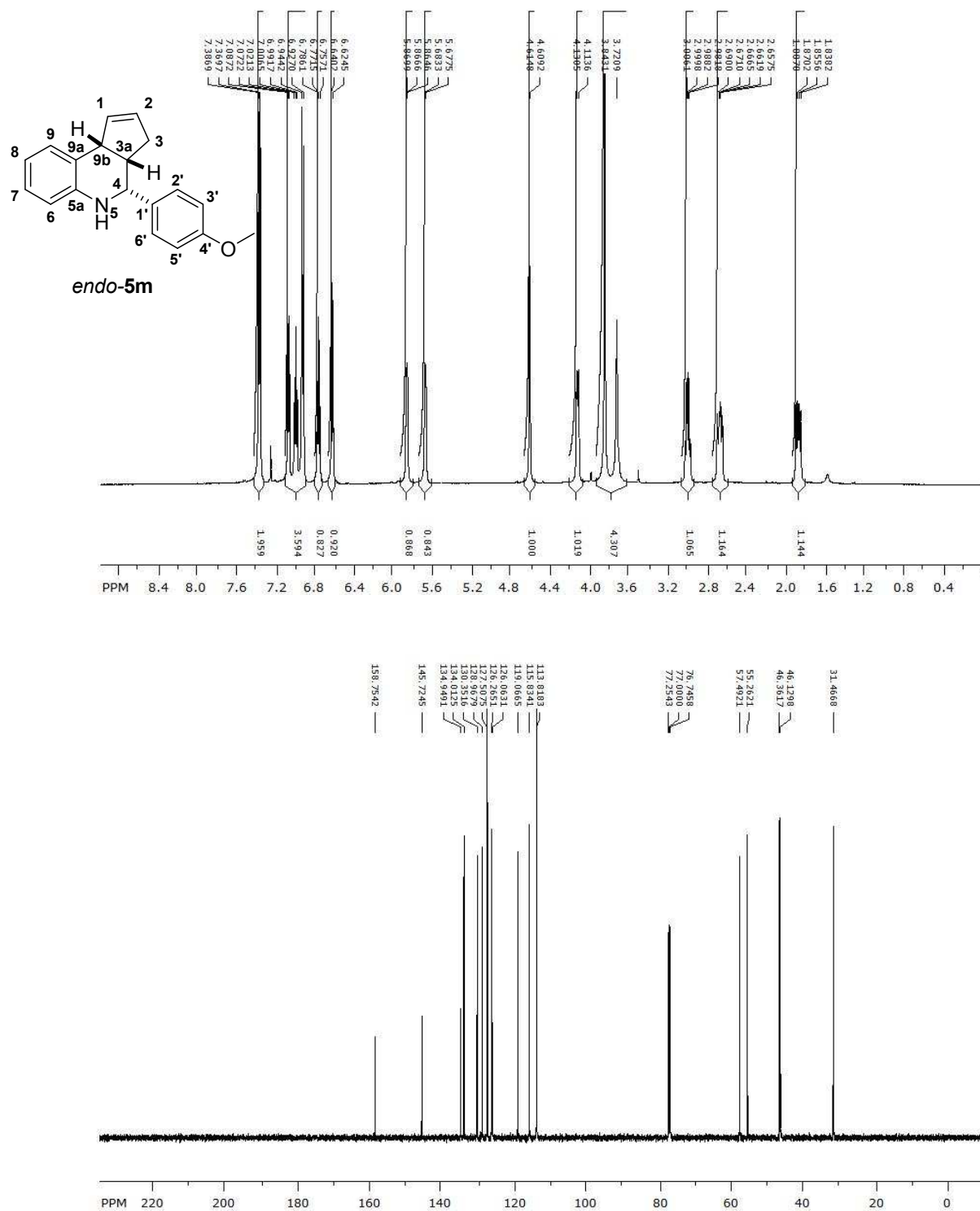


Figure 15. ¹H (300 MHz) and ¹³C (75 MHz) NMR spectra of *endo*-5*m* in CDCl₃.

(3a*SR*,4*RS*,9b*RS*)-4-*p*-Tolyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5n**)

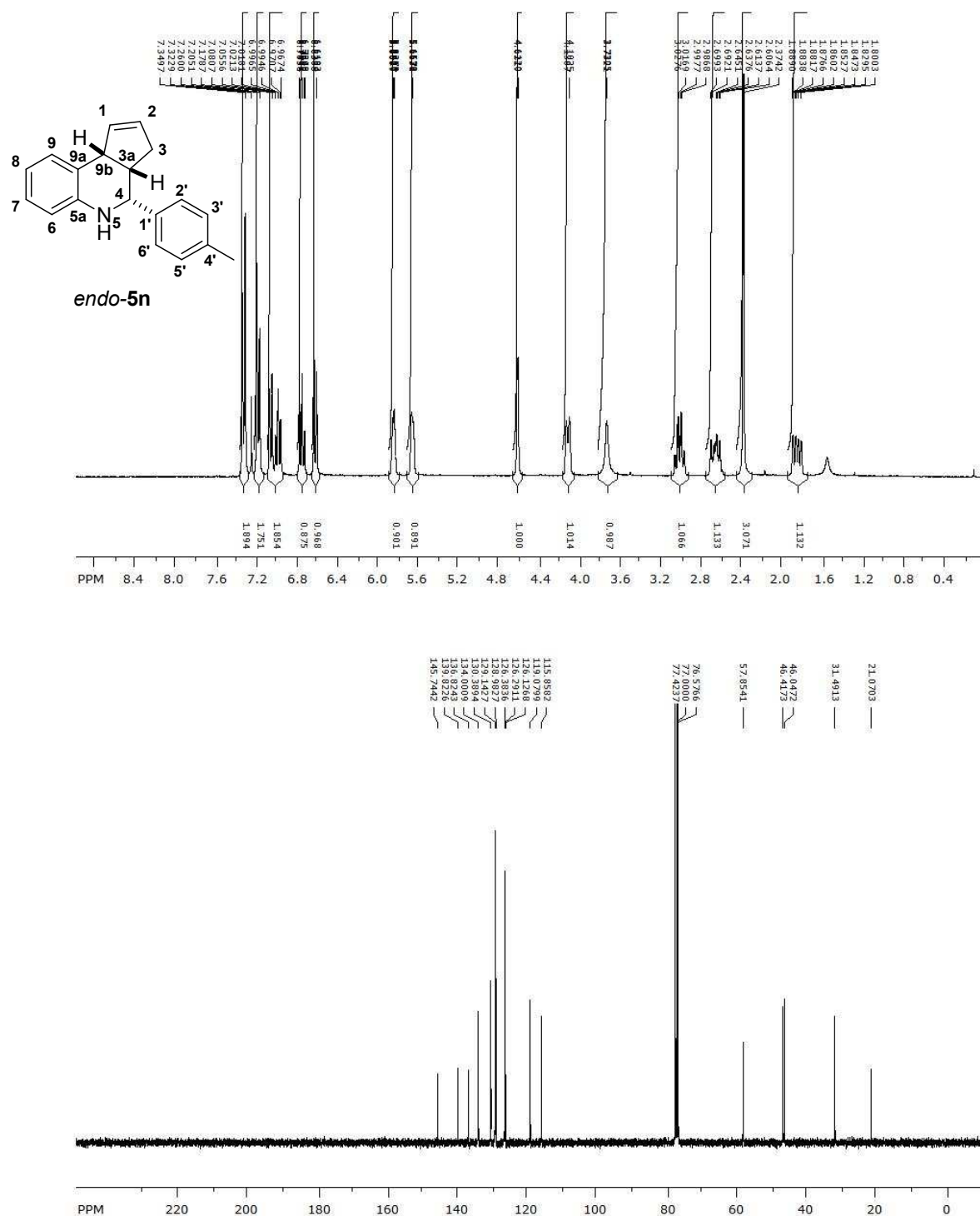


Figure 16. ¹H (300 MHz) and ¹³C (75 MHz) NMR spectra of *endo*-**5n** in CDCl₃.

(3a*SR*,4*RS*,9b*RS*)-4-(Pyridin-3-yl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5o**)

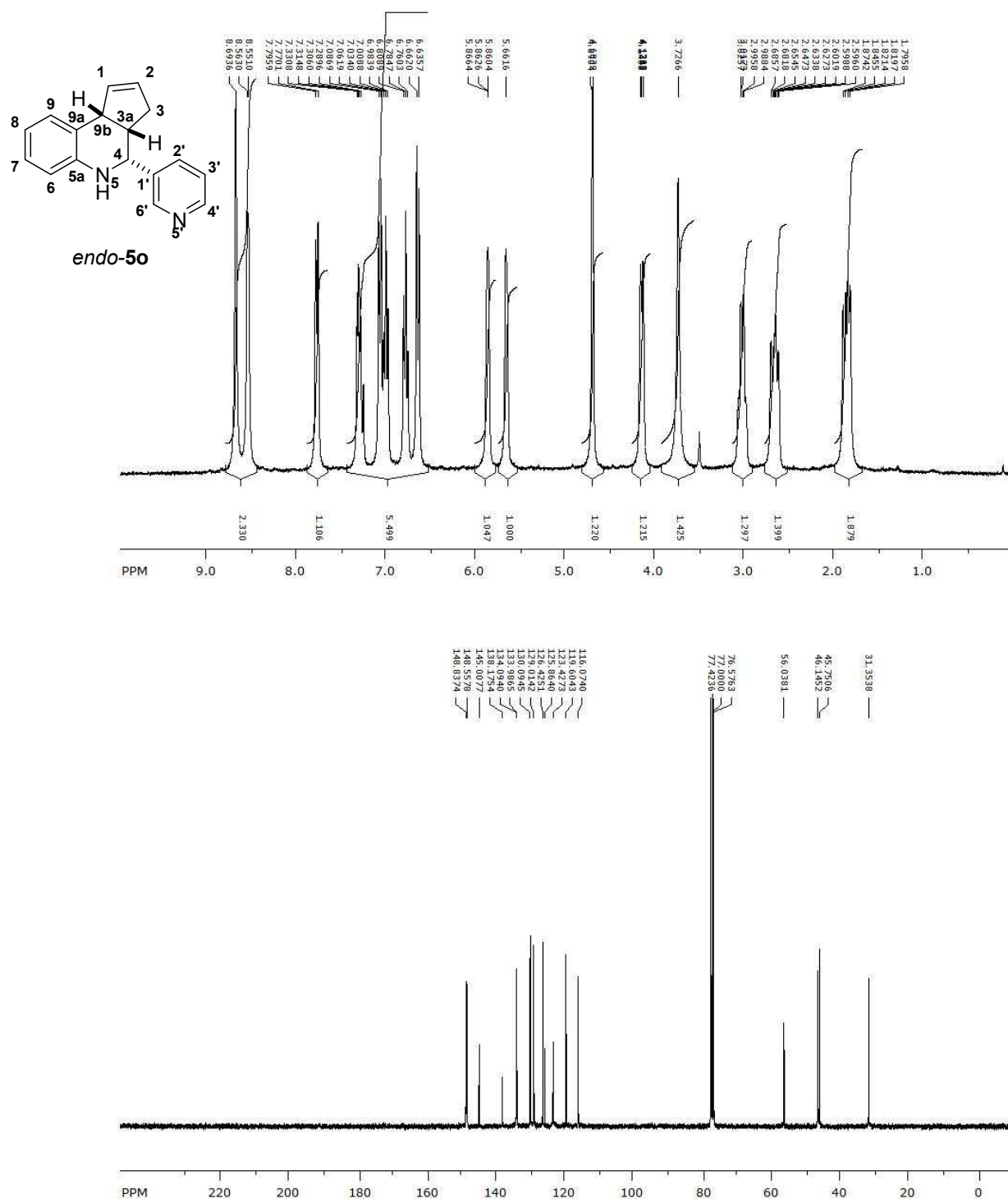


Figure 17. ¹H (300 MHz) and ¹³C (75 MHz) NMR spectra of *endo*-**5o** in CDCl₃.

(3a*SR*,4*RS*,9b*RS*)-4-(Furan-2-yl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5p**)

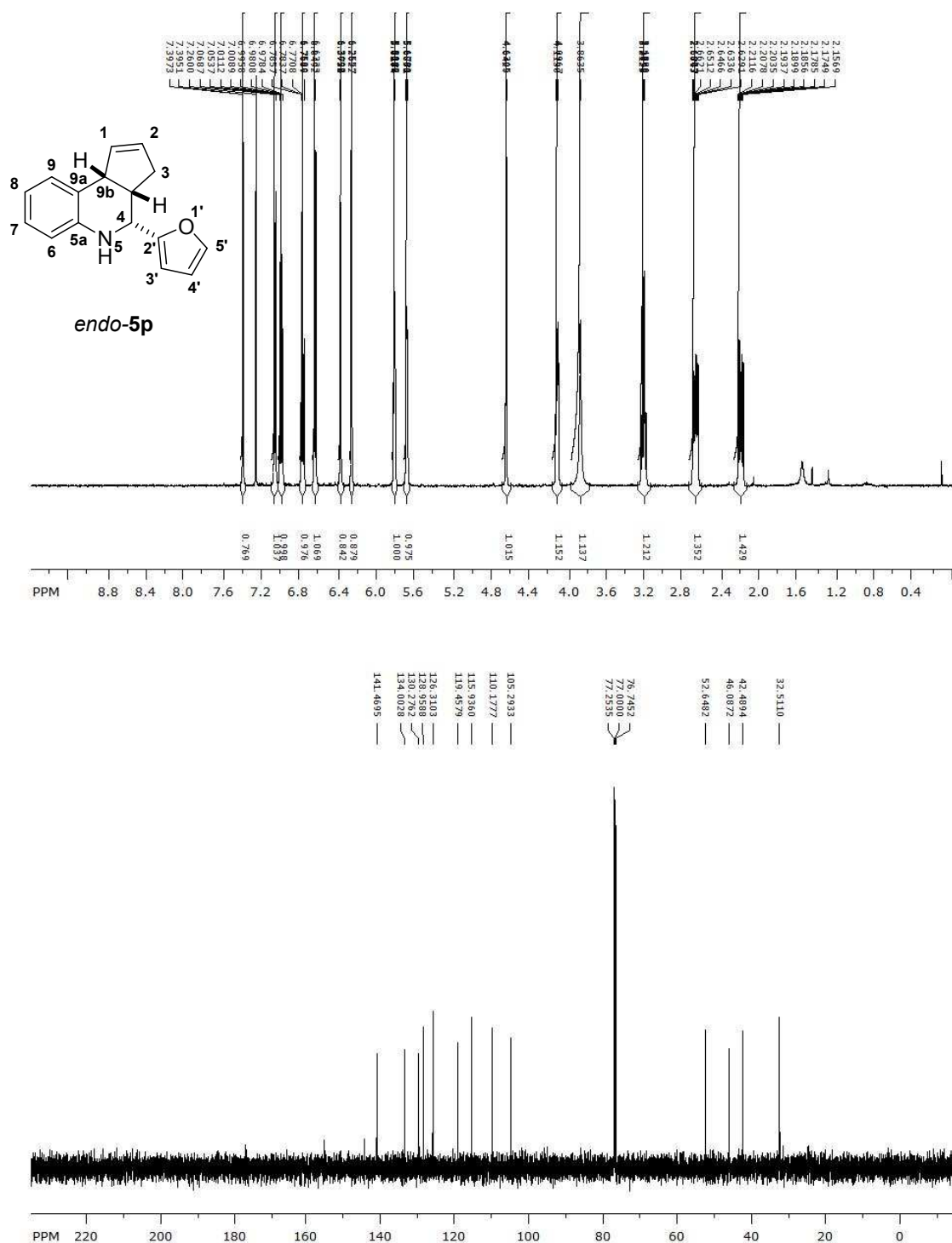


Figure 18. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-**5p** in CDCl₃.

(3a*SR*,4*RS*,9b*RS*)-4-Cyclohexyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5q**)

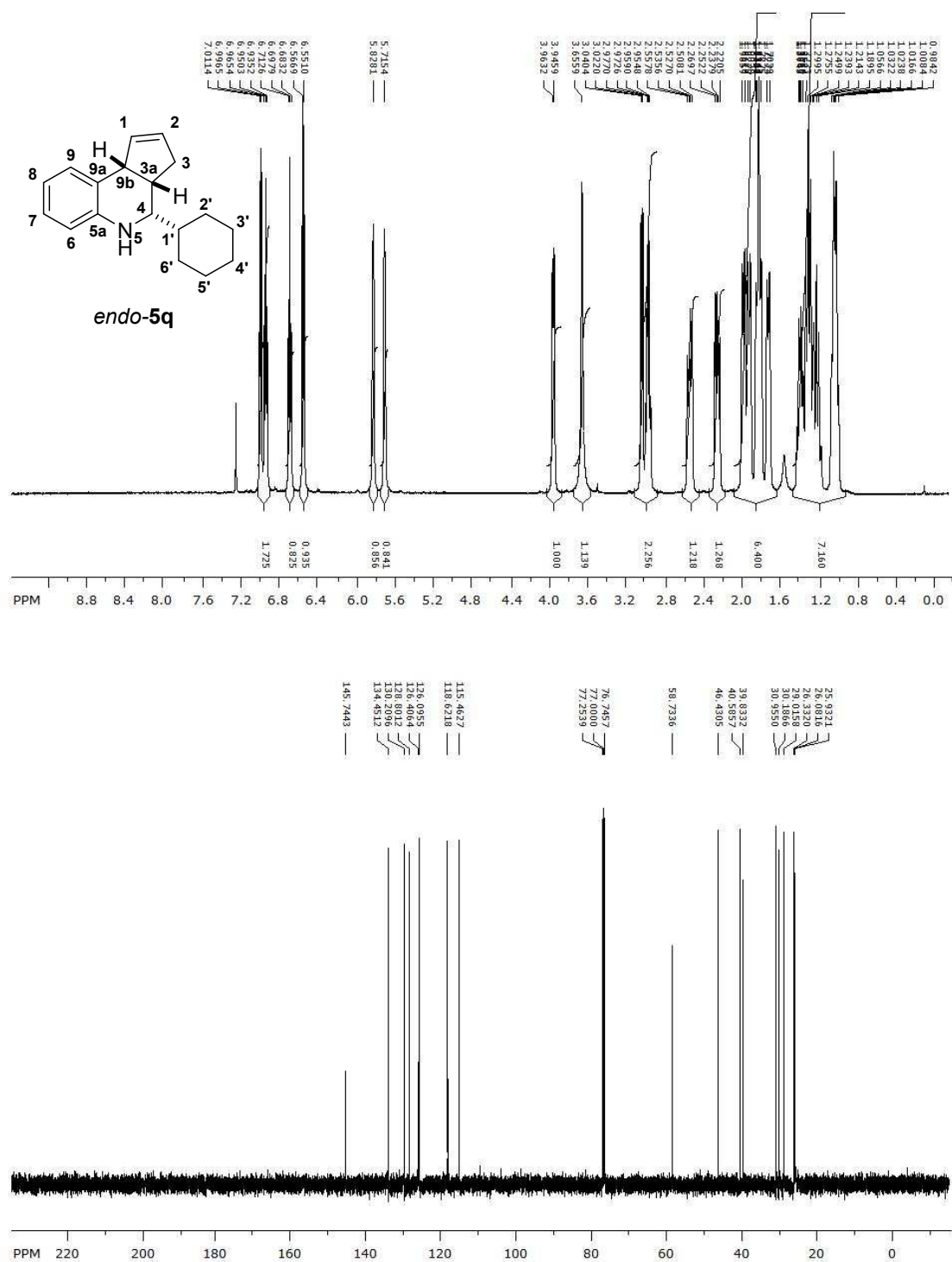


Figure 19. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of *endo*-**5q** in CDCl₃.

(3a*SR*,4*RS*,9b*RS*)-4-*Tert*-butyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (*endo*-**5r**)

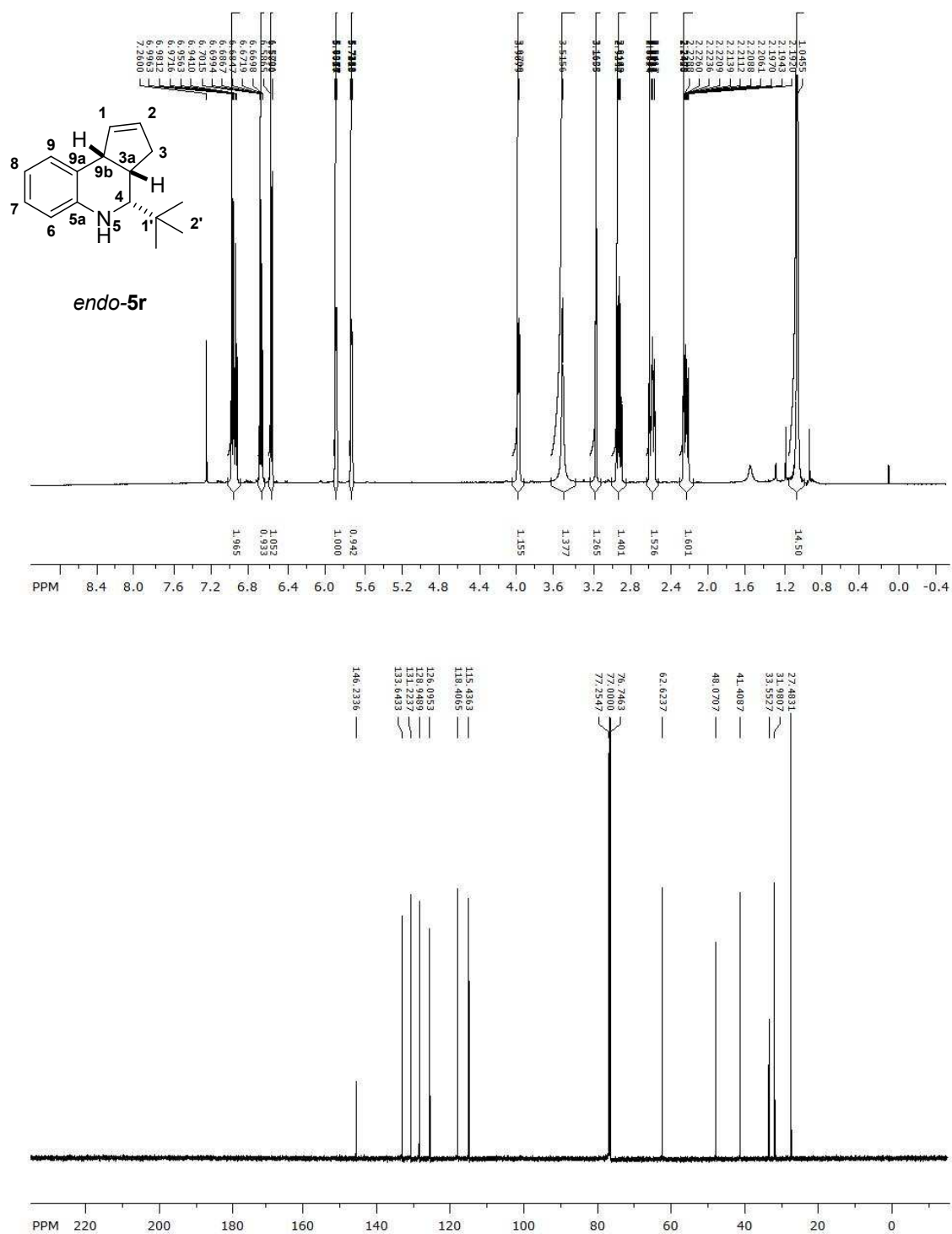


Figure 20. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra of *endo-5r* in CDCl_3 .

(2*SR*,4*RS*)-2,4-Diphenyl-1,2,3,4-tetrahydroquinoline (**8**)

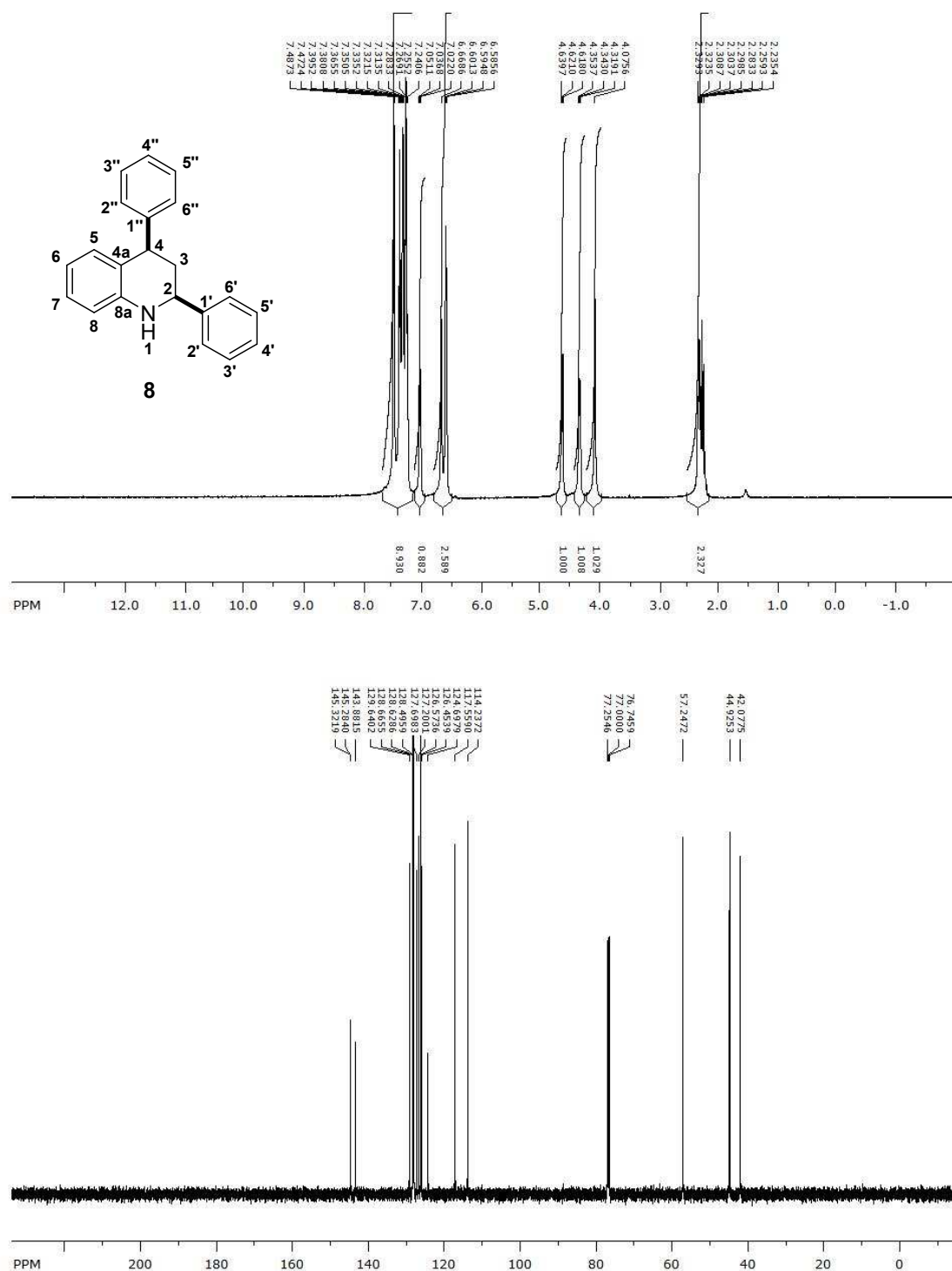


Figure 21. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra of **8** in CDCl_3 .

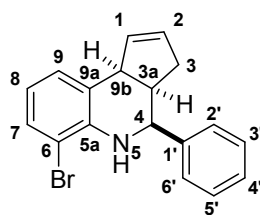
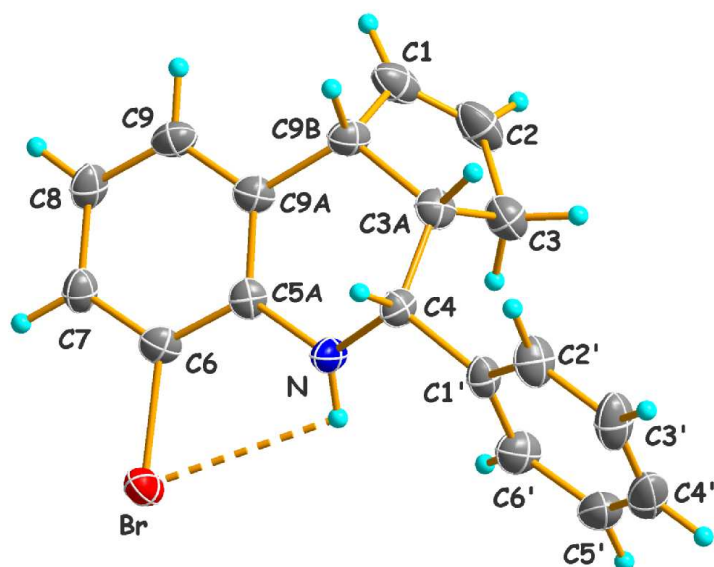


Figure 22. X-ray crystal structure of (3a*SR*,4*RS*,9b*RS*)-6-bromo-4-phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (**5b**)

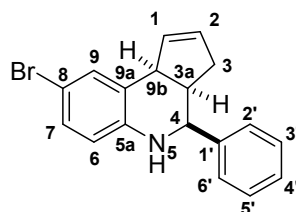
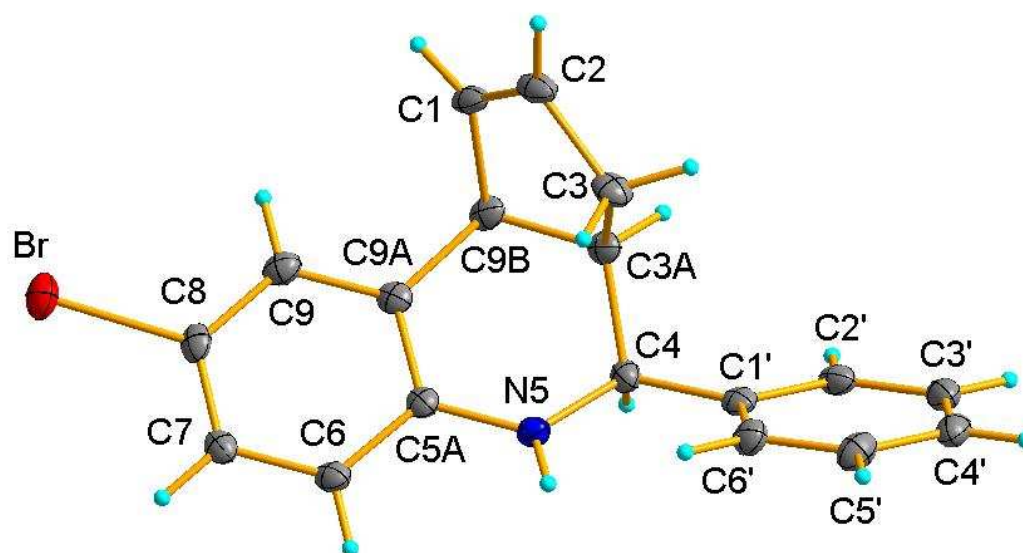


Figure 23. X-ray crystal structure of (3a*SR*,4*RS*,9b*RS*)-8-bromo-4-phenyl-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (**5d**)

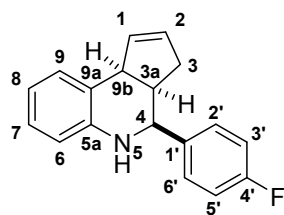
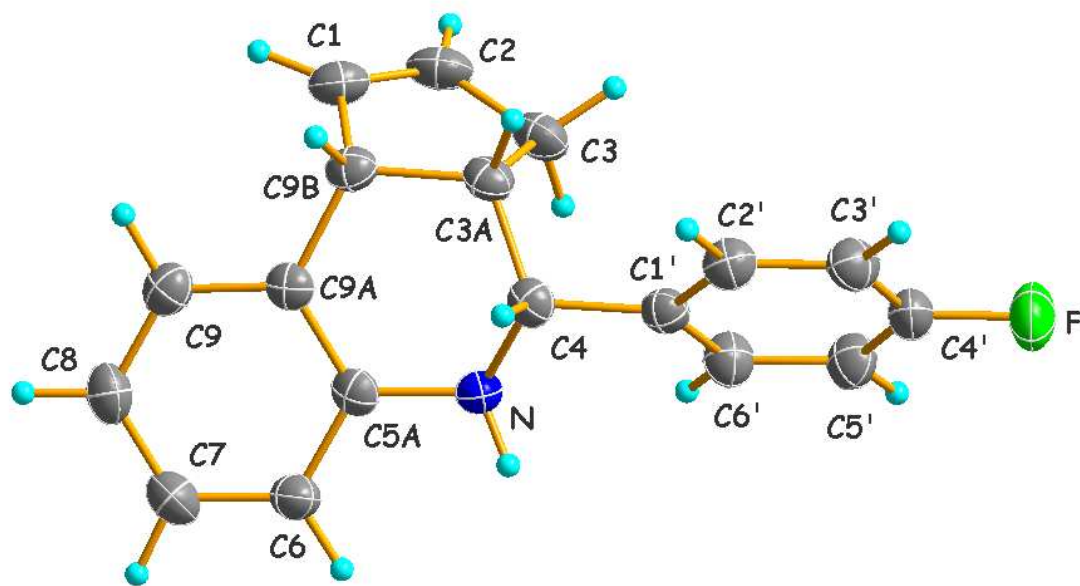


Figure 24. X-ray crystal structure of (3a*SR*,4*RS*,9b*RS*)-4-(4-fluorophenyl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinoline (**5h**)