Sesquiterpenoids and Phenylpropanoids from Chloranthus serratus

Tao Yuan, Chuan-Rui Zhang, Sheng-Ping Yang, Sheng Yin, Wen-Bin Wu, Lei Dong and Jian-Min Yue

State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, 555 Zu Chong Zhi Road, Zhangjiang Hi-Tech Park, Shanghai, 201203, People's Republic of China

Supporting Information Available

Figure S1. Selected HMBC and ROESY correlations of 1-9

For Compound 1

Figure S2. ¹H NMR spectrum of Chlorantene **A** (1) in CDCl₃

Figure S3. ¹³C NMR spectrum of Chlorantene A (1) in CDCl₃

Figure S4. HSQC spectrum of Chlorantene A (1) in CDCl₃

For Compound 2

Figure S5. ¹H NMR spectrum of Chlorantene **B** (2) in CDCl₃

Figure S6. ¹³C NMR spectrum of Chlorantene **B** (2) in CDCl₃

Figure S7. HSQC spectrum of Chlorantene **B** (2) in CDCl₃

For Compound 3a

Figure S8. ¹H NMR spectrum of Compound **3a** in CDCl₃

Figure S9. ¹H NMR spectrum of Compound **3a** in DMSO-d₆

Figure S10. ¹³C NMR spectrum of Compound **3a** in CDCl₃

Figure S11. 13 C NMR spectrum of Compound **3a** in DMSO- d_6

Figure S12. HSQC spectrum of Compound 3a in CDCl₃

For Compound 3

Figure S13. ¹H NMR spectrum of Chlorantene C (3) in CDCl₃

Figure S14. ¹H NMR spectrum of Chlorantene C (3) in DMSO- d_6

Figure S15. ¹³C NMR spectrum of Chlorantene C (3) in CDCl₃

Figure S16. 13 C NMR spectrum of Chlorantene C (3) in DMSO- d_6

Figure S17. HSQC spectrum of Chlorantene C (3) in CDCl₃

For Compound 4

Figure S18. ¹H NMR spectrum of Chlorantene **D** (4) in CD₃COCD₃

Figure S19. ¹³C NMR spectrum of Chlorantene **D** (4) in CD₃COCD₃

Figure S20. HSQC spectrum of Chlorantene **D** (4) in CD₃COCD₃

For Compound **5**

Figure S21. ¹H NMR spectrum of Chlorantene **E** (**5**) in CDCl₃

Figure S22. ¹³C NMR spectrum of Chlorantene **E** (**5**) in CDCl₃

For Compound 6

Figure S23. ¹H NMR spectrum of Chlorantene **F** (**6**) in CDCl₃

Figure S24. ¹³C NMR spectrum of Chlorantene **F** (6) in CDCl₃

For Compound 7

Figure S25. ¹H NMR spectrum of Chlorantene **G** (7) in CDCl₃

Figure S26. ¹³C NMR spectrum of Chlorantene **G** (**7**) in CDCl₃

Figure S27. HSQC spectrum of Chlorantene G (7) in CDCl₃

For Compound 8 and 9

Figure S28. ¹H NMR spectrum of compound **8** in CDCl₃

Figure S29. ¹H NMR spectrum of compound **9** in CDCl₃

Figure S30. ¹³C NMR spectrum of compound **8** in CDCl₃

Figure S31. ¹³C NMR spectrum of compound **9** in CDCl₃

Figure S1. Selected HMBC and ROESY correlations of 1-9

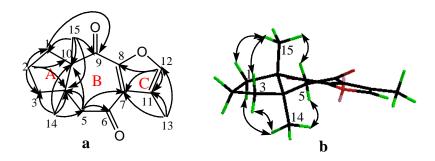


Figure 1. Selected HMBC (H \rightarrow C) (a) and ROESY (\leftrightarrow) (b) correlations of chlorantene A (1)

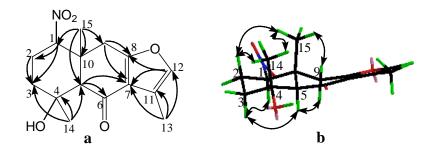


Figure 2. Selected HMBC (H \rightarrow C) (a) and ROESY (\leftrightarrow) (b) correlations of chlorantene B (2)

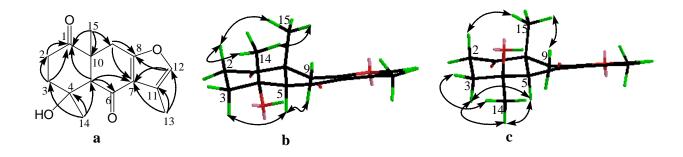


Figure 3. Selected HMBC (H \rightarrow C) of compounds 3 and 3a (a); Selected ROESY (\leftrightarrow) correlations of 3a (b) and 3 (c)

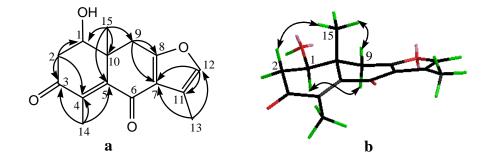


Figure 4. Selected HMBC (H \rightarrow C) (a) and ROESY (\leftrightarrow) (b) correlations of chlorantene D (4)

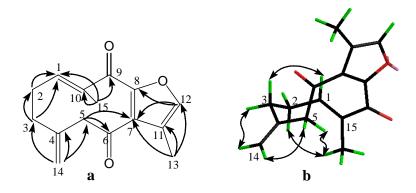


Figure 5. Selected HMBC (H \rightarrow C) (a) and ROESY (\leftrightarrow) (b) correlations of chlorantene E (5)

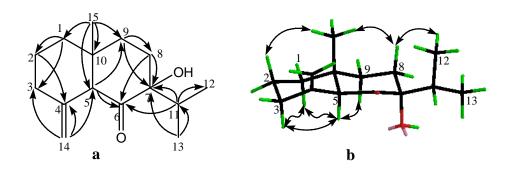


Figure 6. Selected HMBC (H \rightarrow C) (a) and ROESY (\leftrightarrow) (b) correlations of chlorantene G (7)

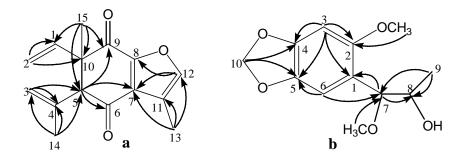


Figure 7. Selected HMBC (H→C) correlations of chlorantene F (6) (a) and compounds 8 and 9 (b)

Figure S2. ¹H NMR spectrum of Chlorantene **A** (1) in CDCl₃

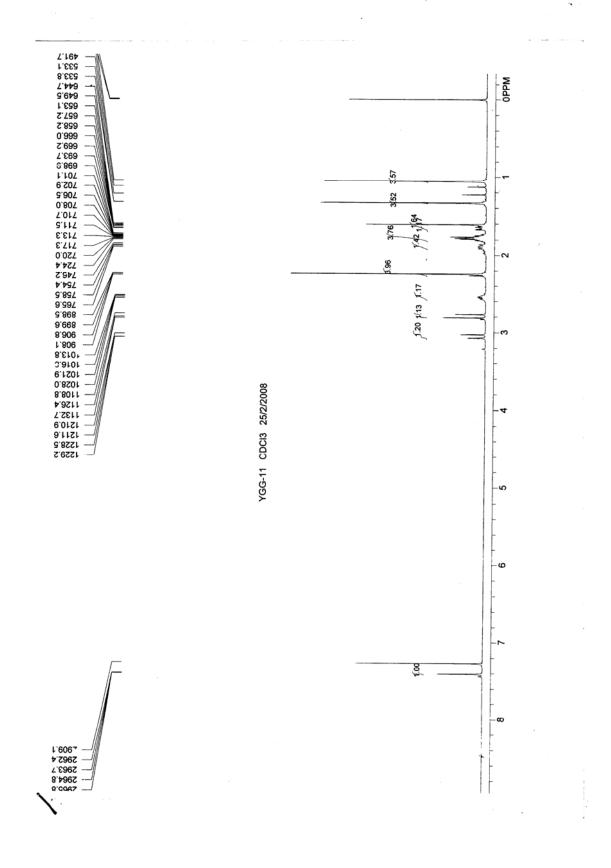


Figure S3. ¹³C NMR spectrum of Chlorantene **A** (1) in CDCl₃

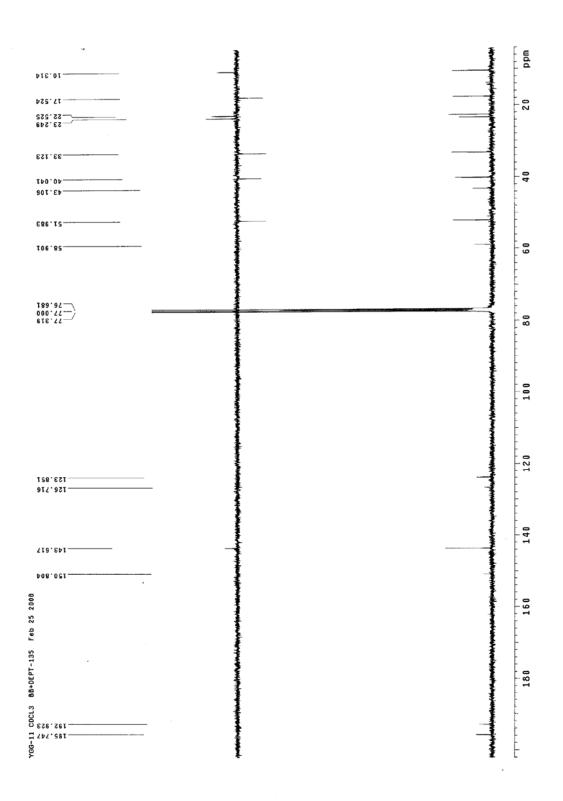


Figure S4. HSQC spectrum of Chlorantene A (1) in CDCl₃

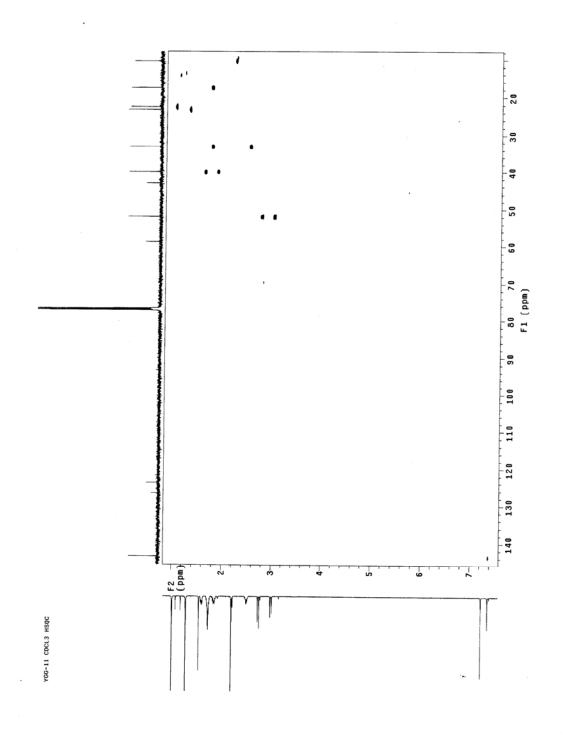


Figure S5. ¹H NMR spectrum of Chlorantene **B** (2) in CDCl₃

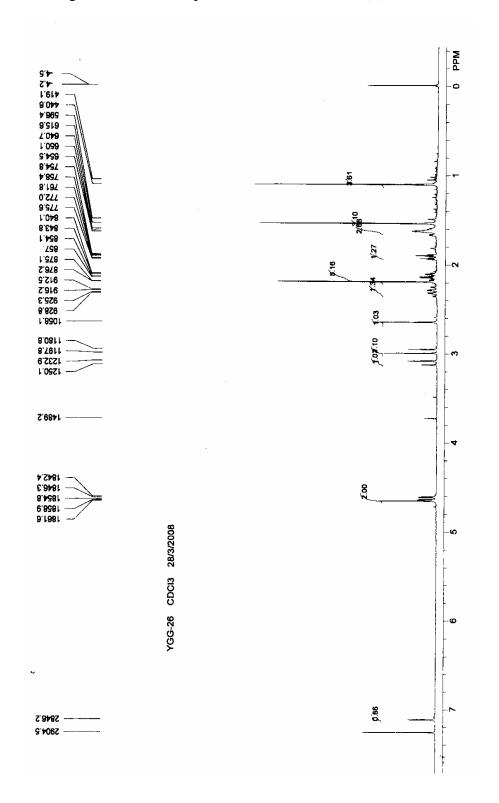


Figure S6. ¹³C NMR spectrum of Chlorantene **B** (2) in CDCl₃

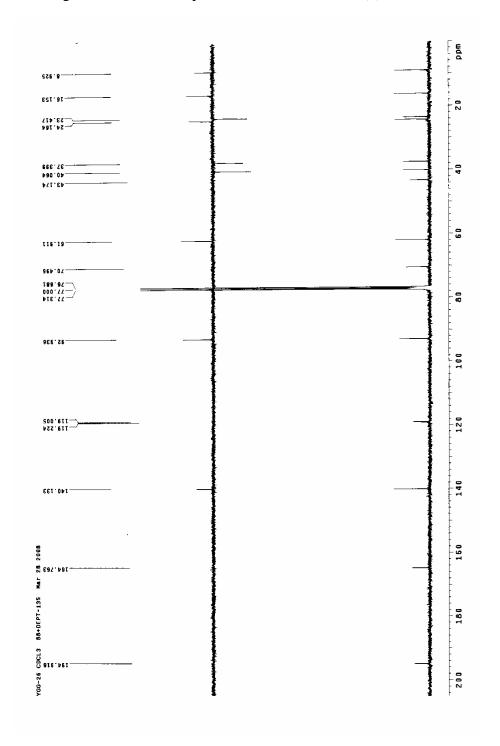


Figure S7. HSQC spectrum of Chlorantene **B** (2) in CDCl₃

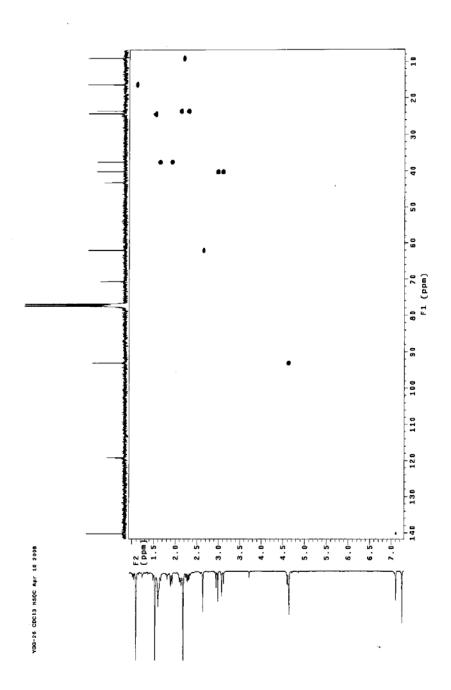


Figure S8. ¹H NMR spectrum of Compound **3a** in CDCl₃

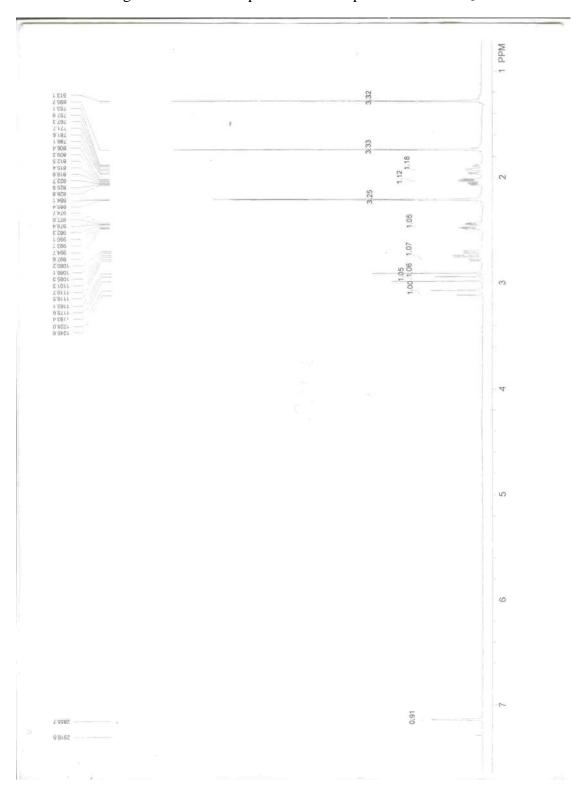


Figure S9. ¹H NMR spectrum of Compound **3a** in DMSO-d₆

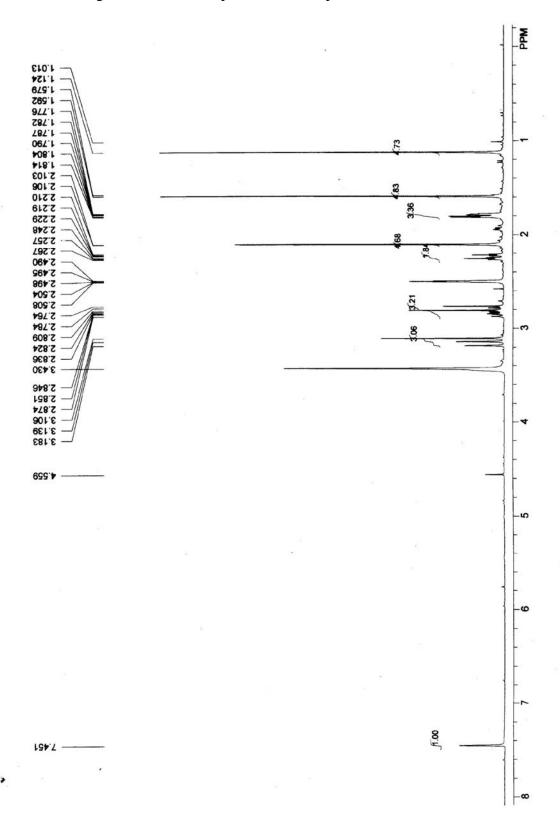


Figure S10. ¹³C NMR spectrum of Compound **3a** in CDCl₃

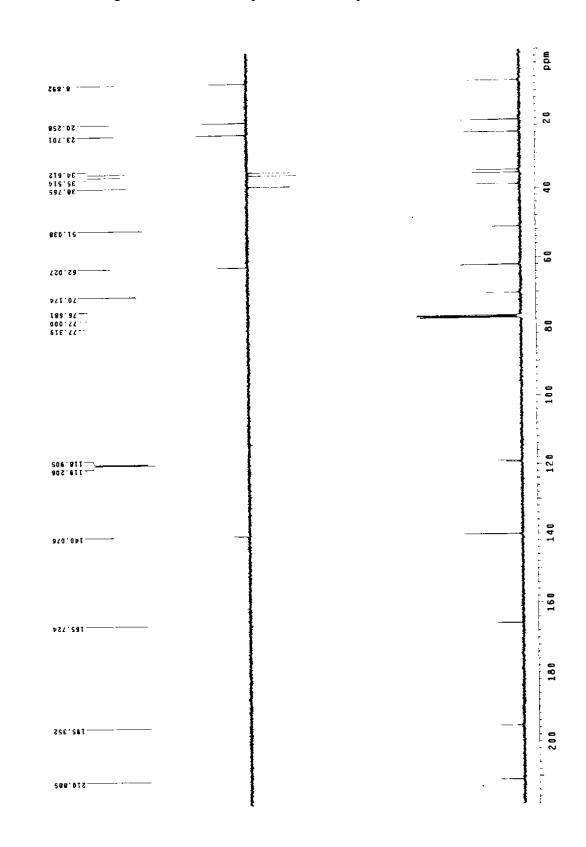


Figure S11. 13 C NMR spectrum of Compound **3a** in DMSO- d_6

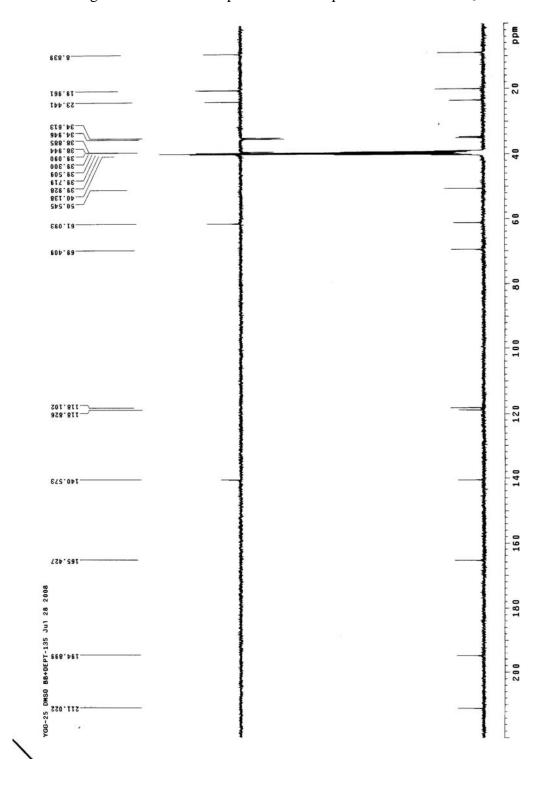


Figure S12. HSQC spectrum of Compound ${\bf 3a}$ in CDCl $_3$

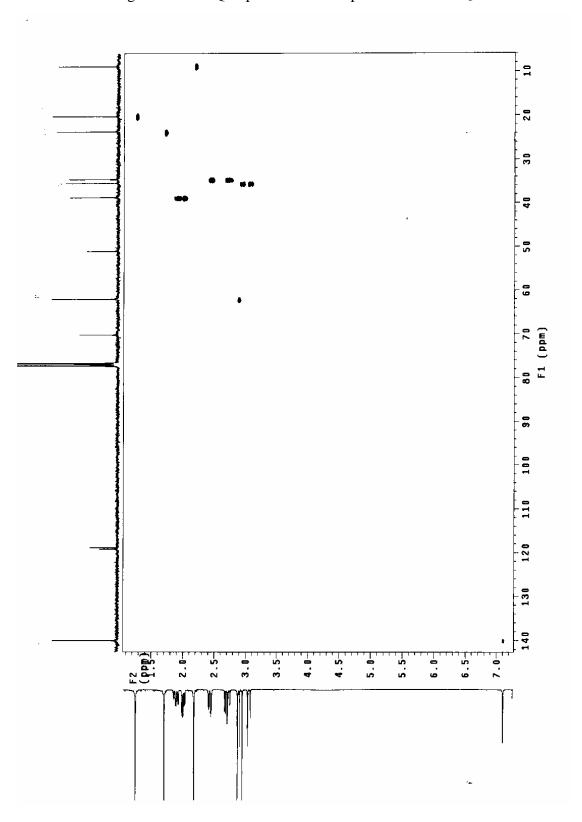


Figure S13. 1 H NMR spectrum of Chlorantene C (3) in CDCl $_{3}$

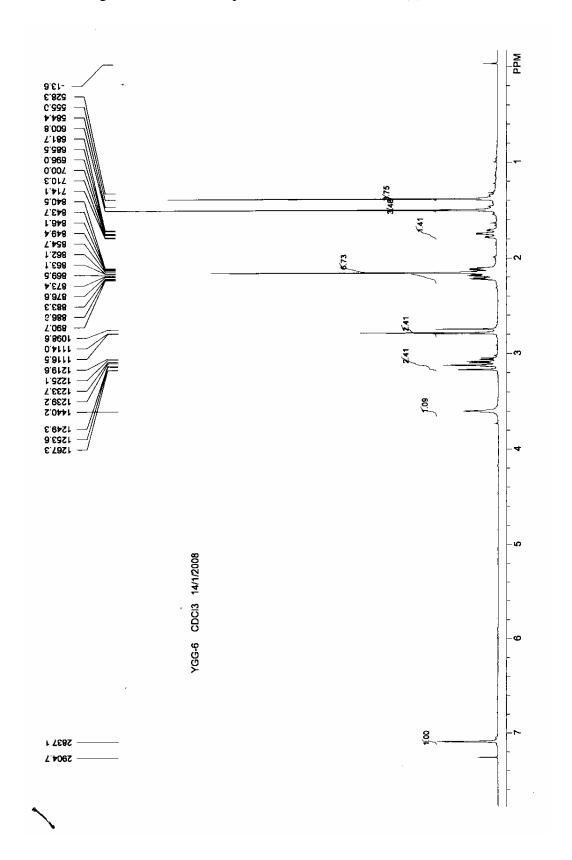


Figure S14. 1 H NMR spectrum of Chlorantene C (3) in DMSO- d_{6}

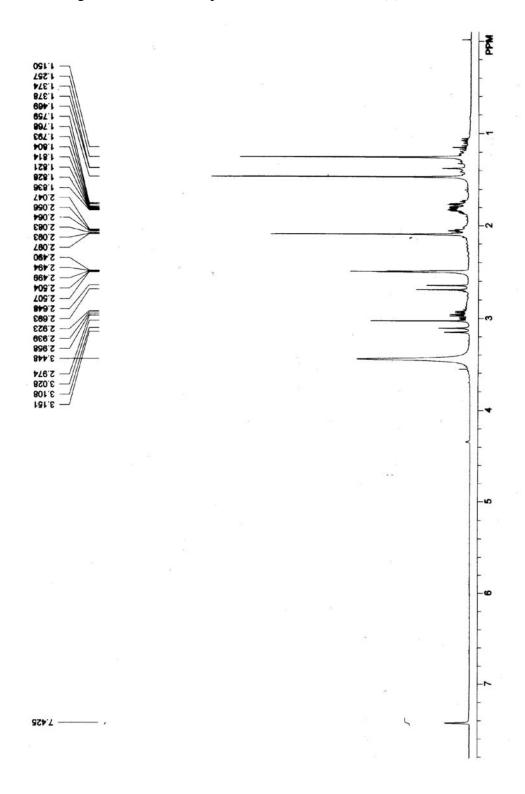


Figure S15. 13 C NMR spectrum of Chlorantene C (3) in CDCl₃

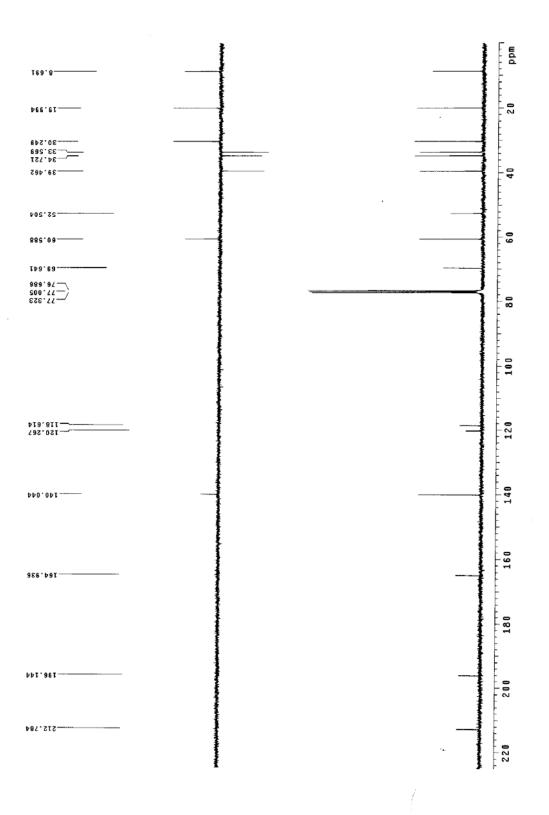


Figure S16. 13 C NMR spectrum of Chlorantene C (3) in DMSO- d_6

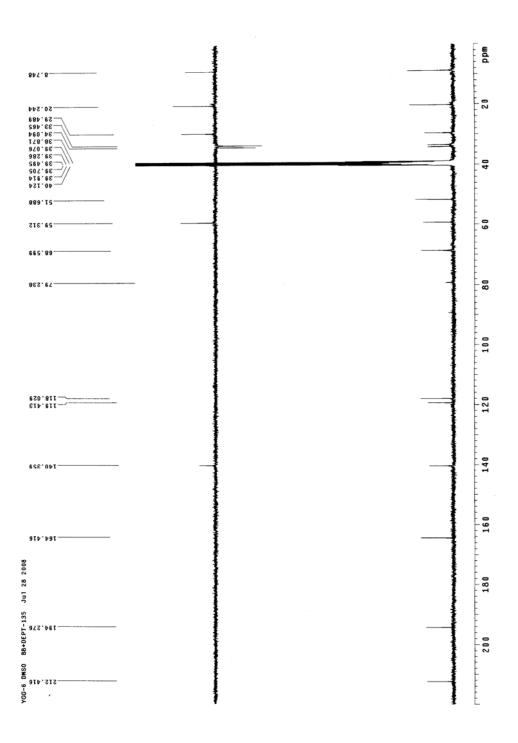


Figure S17. HSQC spectrum of Chlorantene ${\bf C}$ (3) in CDCl₃

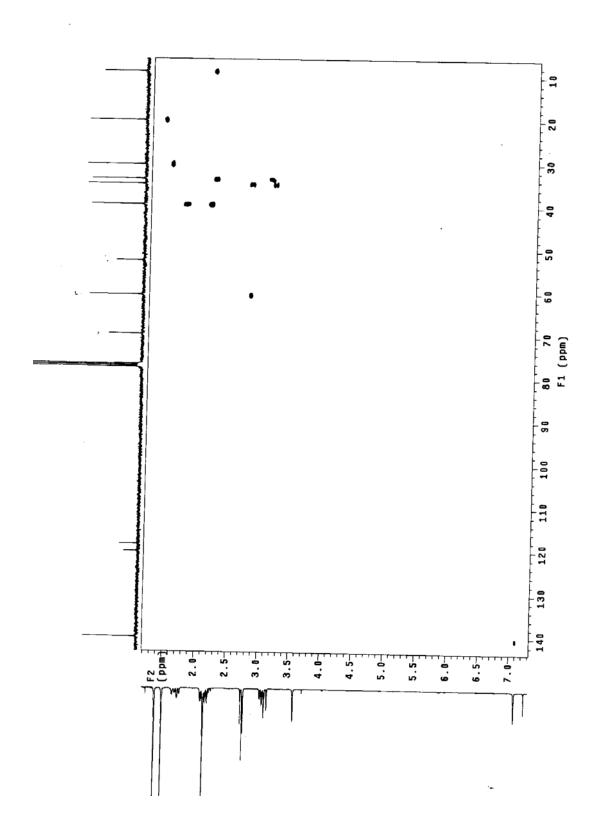


Figure S18. ¹H NMR spectrum of Chlorantene **D** (4) in CD₃COCD₃

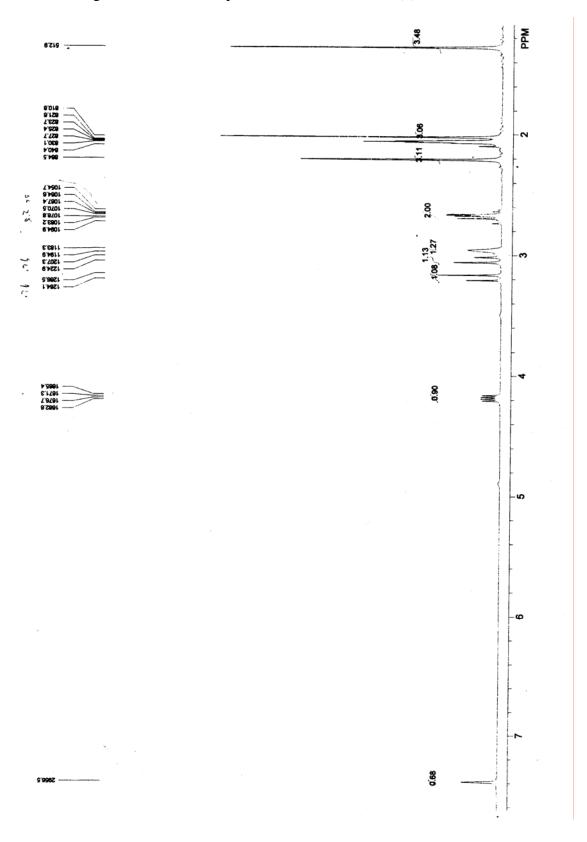


Figure S19. ¹³C NMR spectrum of Chlorantene **D** (4) in CD₃COCD₃

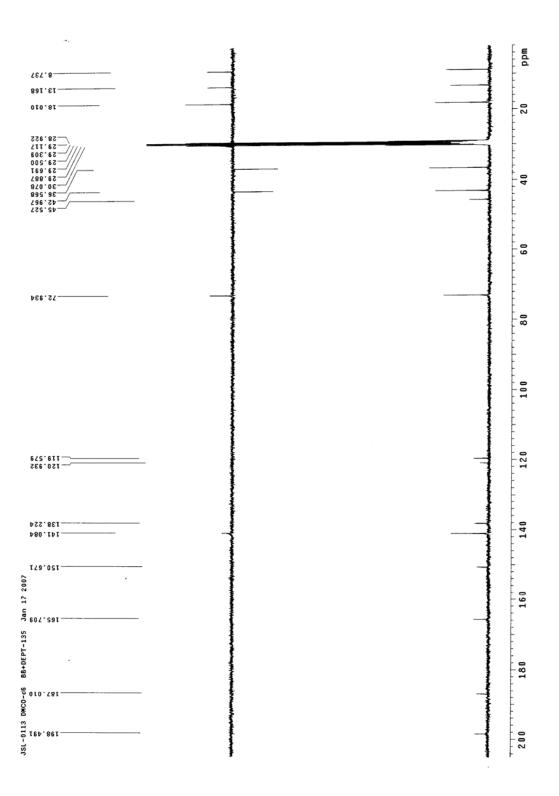


Figure S20. HSQC spectrum of Chlorantene ${\bf D}$ (4) in CD₃COCD₃

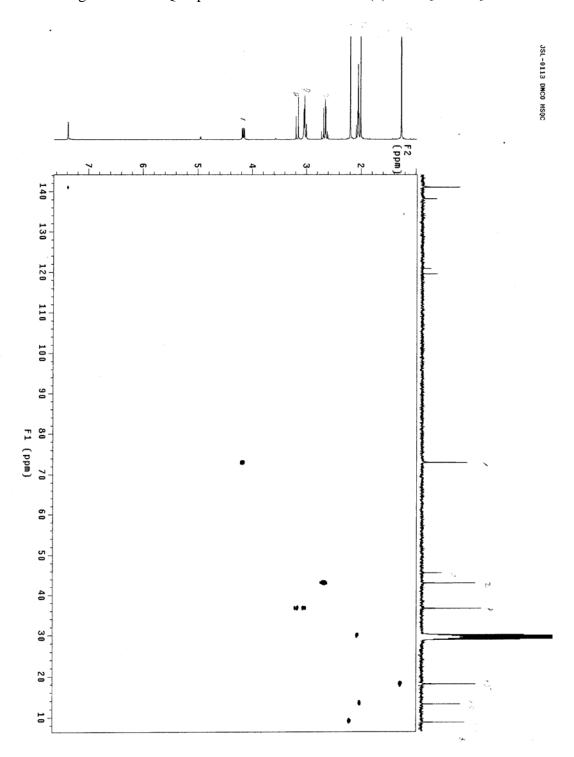


Figure S21. ¹H NMR spectrum of Chlorantene **E** (**5**) in CDCl₃

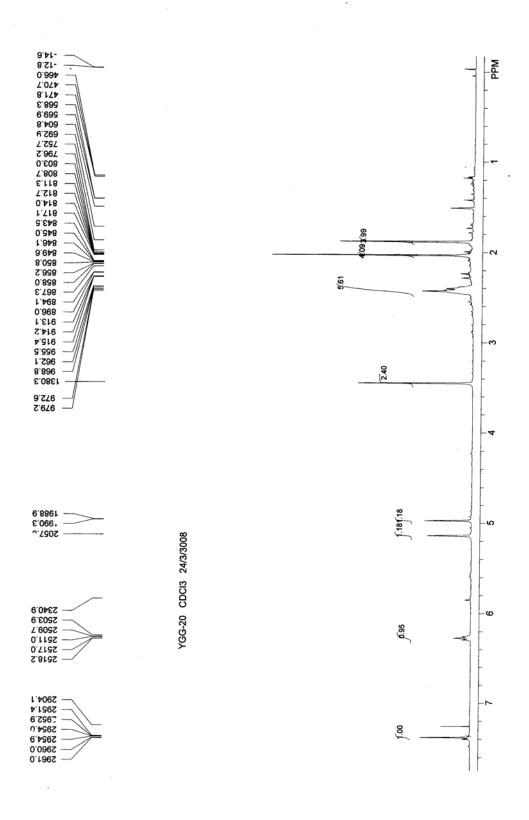


Figure S22. ¹³C NMR spectrum of Chlorantene **E** (**5**) in CDCl₃

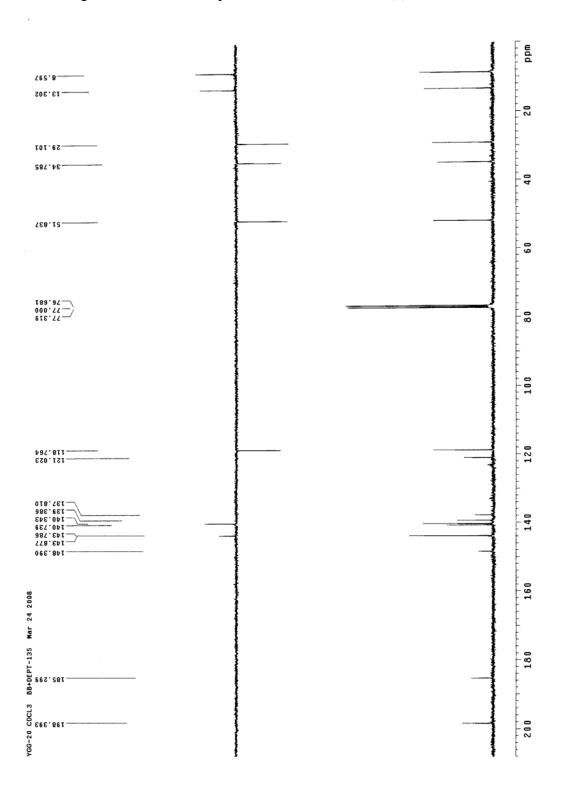


Figure S23. ¹H NMR spectrum of Chlorantene **F** (**6**) in CDCl₃

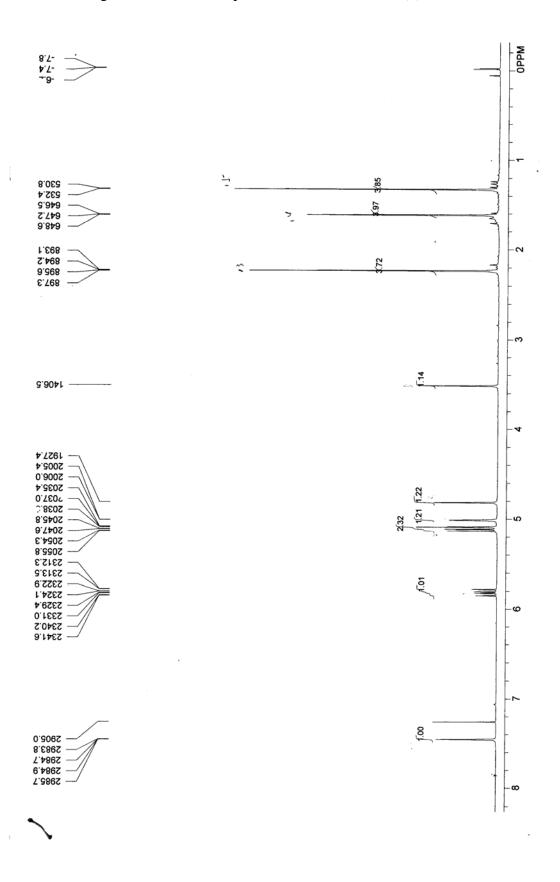


Figure S24. ¹³C NMR spectrum of Chlorantene **F** (**6**) in CDCl₃

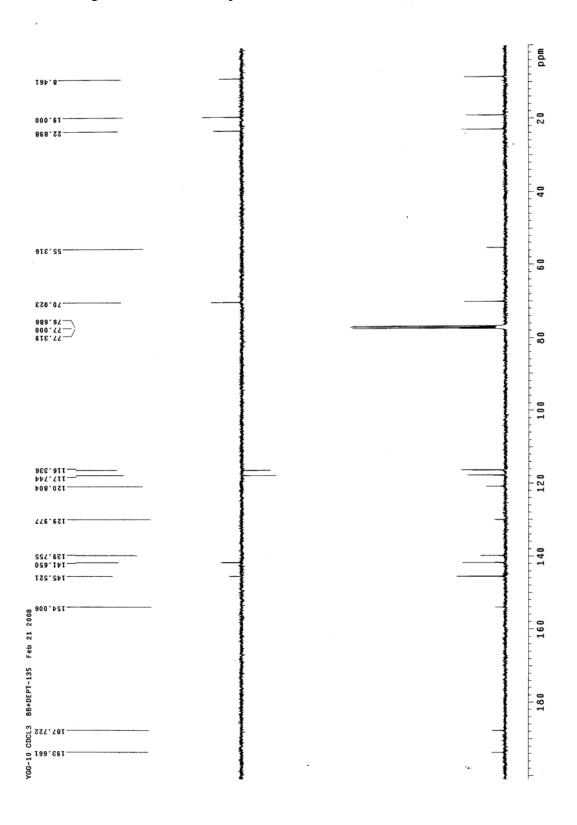


Figure S25. ¹H NMR spectrum of Chlorantene **G** (7) in CDCl₃

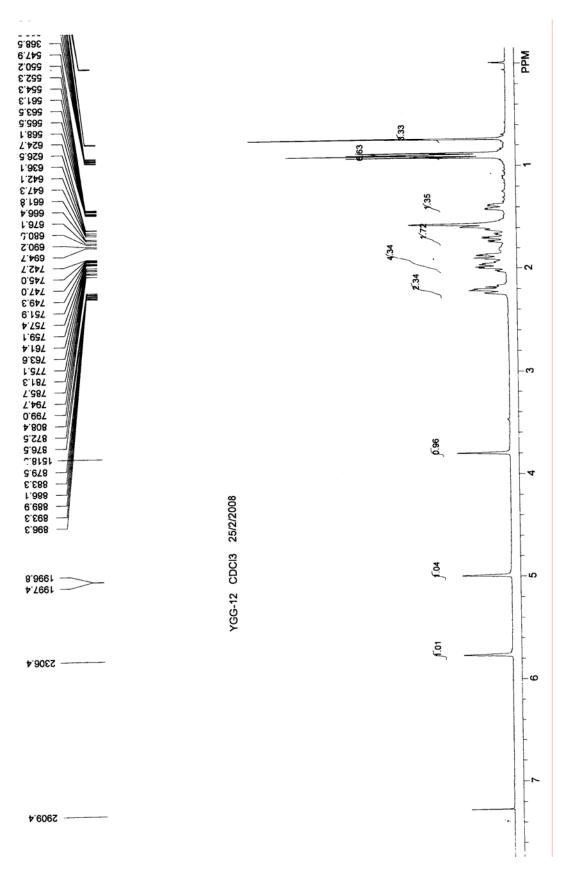


Figure S26. 13 C NMR spectrum of Chlorantene **G** (**7**) in CDCl₃

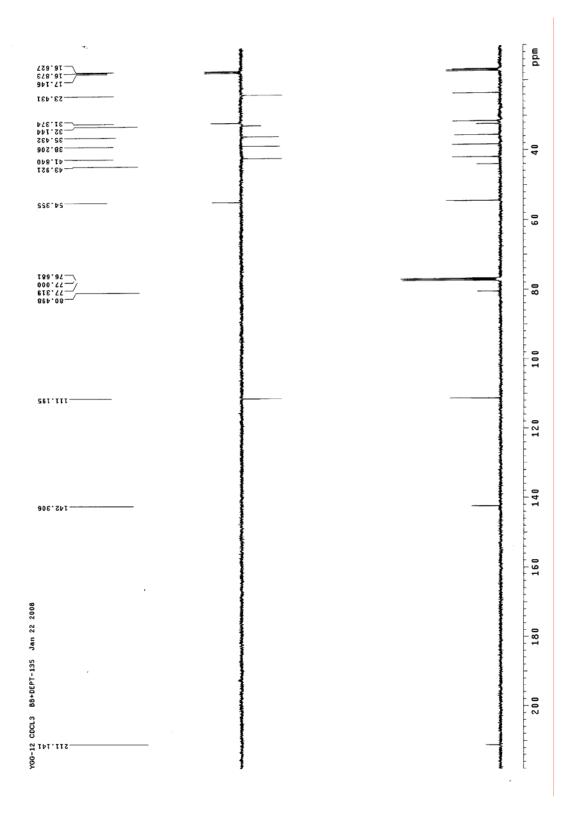


Figure S27. HSQC spectrum of Chlorantene \mathbf{G} (7) in CDCl₃

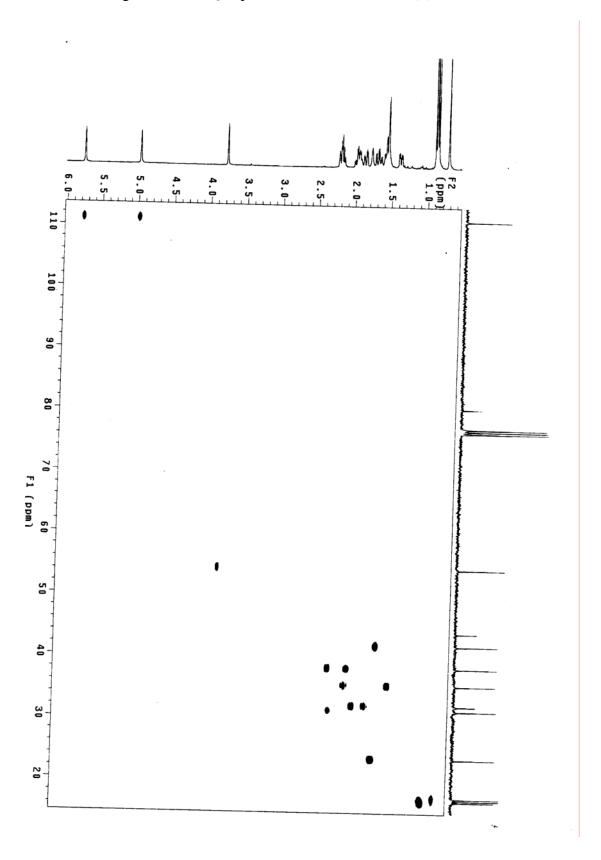


Figure S28. ¹H NMR spectrum of compound **8** in CDCl₃

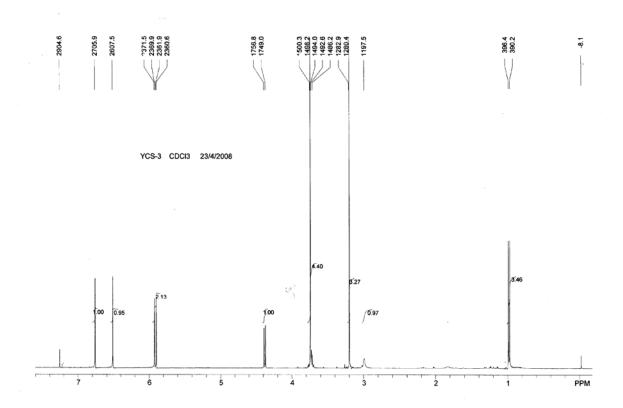


Figure S29. ¹H NMR spectrum of compound **9** in CDCl₃

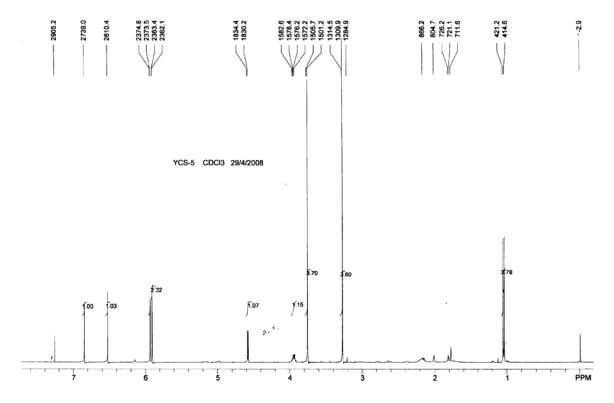


Figure S30. ¹³C NMR spectrum of compound **8** in CDCl₃

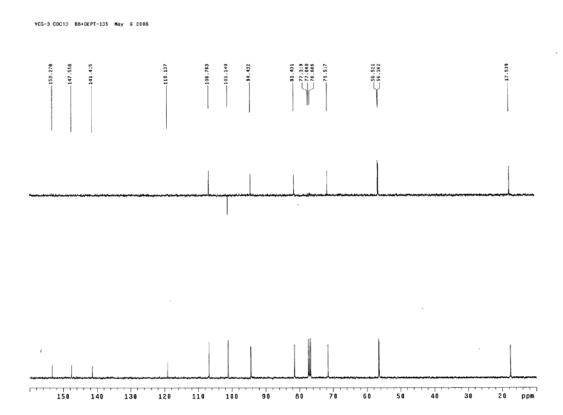


Figure S31. ¹³C NMR spectrum of compound **9** in CDCl₃

