Neo-Clerodane Diterpenoids and other Constituents of Salvia filipes

Emma Maldonado,* Leonel Galicia, Ma. Isabel Chávez and Simón Hernández-Ortega

Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Coyoacán, 04510, D. F., México.

All the NMR spectra were recorded on a Varian Inova 500 (¹H at 500 MHz; ¹³C at 125 MHz, using TMS as internal standard)

Figure S1. ¹H NMR spectrum of compound **1**(CDCl₃)

Figure S2. ¹³C NMR spectrum of compound 1 (CDCl₃)

Figure S3. COSY spectrum of compound 1 (CDCl₃)

Figure S4. HSQC spectrum of compound 1 (CDCl₃)

Figure S5. HMBC spectrum of compound 1 (CDCl₃)

Figure S6. NOESY spectrum of compound 1 (CDCl₃)

Figure S7. ¹H NMR spectrum of compound 3 (DMSO-d₆)
Figure S8 ¹³C NMR spectrum of compound 3 (DMSO-d₆)
Figure S9. COSY spectrum of compound 3 (DMSO-d₆)
Figure S10. HSQC spectrum of compound 3 (DMSO-d₆)
Figure S11. HMBC spectrum of compound 3 (DMSO-d₆)
Figure S12. NOESY spectrum of compound 3 (DMSO-d₆)

Figure S13. ¹H NMR spectrum of compound 4/5 (CDCl₃)
Figure S14. ¹³C NMR spectrum of compound 4/5 (CDCl₃)
Figure S15. COSY spectrum of compound 4/5 (CDCl₃)
Figure S16. HSQC spectrum of compound 4/5 (CDCl₃)
Figure S17. HMBC spectrum of compound 4/5 (CDCl₃)
Figure S18. NOESY spectrum of compound 4/5 (CDCl₃)

Figure S19. ¹H NMR spectrum of compound 7 (DMSO-d₆)
Figure S20 ¹³C NMR spectrum of compound 7 (DMSO-d₆)
Figure S21. COSY spectrum of compound 7 (DMSO-d₆)
Figure S22. HSQC spectrum of compound 7 (DMSO-d₆)
Figure S23. HMBC spectrum of compound 7 (DMSO-d₆)
Figure S24. NOESY spectrum of compound 7 (DMSO-d₆)

Figure S25. ¹H NMR spectrum of compound 8 (DMSO-d₆)
Figure S26 ¹³C NMR spectrum of compound 8 (DMSO-d₆)
Figure S27. COSY spectrum of compound 8 (DMSO-d₆)
Figure S28. HSQC spectrum of compound 8 (DMSO-d₆)
Figure S29. HMBC spectrum of compound 8 (DMSO-d₆)
Figure S30. NOESY spectrum of compound 8 (DMSO-d₆)

 Table S1. ¹H and ¹³C NMR Data of Compound 10



Figure S1. ¹H NMR spectrum of compound 1(CDCl₃)





Figure S3. COSY spectrum of compound 1 (CDCl₃)



Figure S4. HSQC spectrum of compound 1 (CDCl₃)



Figure S5. HMBC spectrum of compound 1 (CDCl₃)



Figure S6. NOESY spectrum of compound 1 (CDCl₃)





Figure S8 ¹³C NMR spectrum of compound 3 (DMSO-d₆)



Figure S9. COSY spectrum of compound **3** (DMSO-d₆)



Figure S10. HSQC spectrum of compound 3 (DMSO-d₆)



Figure S11. HMBC spectrum of compound **3** (DMSO-d₆)



Figure S12. NOESY spectrum of compound **3** (DMSO-d₆)



Figure S13. 1 H NMR spectrum of compound 4/5 (CDCl₃)



Figure S14. ¹³C NMR spectrum of compound 4/5 (CDCl₃)



Figure S15. COSY spectrum of compound 4/5 (CDCl₃)



Figure S16. HSQC spectrum of compound 4/5 (CDCl₃)



Figure S17. HMBC spectrum of compound 4/5 (CDCl₃)



Figure S18. NOESY spectrum of compound 4/5 (CDCl₃)



Figure S19. ¹H NMR spectrum of compound 7 (DMSO-d₆)



Figure S20¹³C NMR spectrum of compound 7 (DMSO-d₆)



Figure S21. COSY spectrum of compound 7 (CDCl₃)



Figure S22. HSQC spectrum of compound 7 (DMSO-d₆)



Figure S23. HMBC spectrum of compound 7 (DMSO-d₆)



Figure S24. NOESY spectrum of compound 7 (DMSO-d₆)



Figure S25. ¹H NMR spectrum of compound 8 (DMSO-d₆)



Figure S26¹³C NMR spectrum of compound 8 (DMSO-d₆)



Figure S27. COSY spectrum of compound 8 (DMSO-d₆)



Figure S28. HSQC spectrum of compound 8 (DMSO-d₆)



Figure S29. HMBC spectrum of compound **8** (DMSO-d₆)



Figure S30. NOESY spectrum of compound 8 (DMSO-d₆)

Position	$^{1}\mathrm{H}$	¹³ C	Position	$^{1}\mathrm{H}$	¹³ C
1	5.86 br d (12.0)	126.9 CH	10	2.25 br s	52.0 CH
2	5.88 m	129.0 CH	11α	2.08 dd (15.5, 1.5)	37.2 CH ₂
3	2.36 m	21.3 CH ₂	11 <i>β</i>	2.74 dd (15.5, 8.0)	
3'	2.13 m		12	5.67 ddd (8.0, 1.5, 1.5)	70.6 CH
4	2.38 dd (13.0, 6.0)	46.4 CH	13		127.3 C
5		41.9 C	14	6.40 m	108.6 CH
6α	1.21 ddd (14.0, 3.0, 3.0)	18.2 CH ₂	15	7.37 m	144.3 CH
6β	1.83 dddd (14.0, 14.0, 4.5, 2.0)		16	7.44 dd (2.0, 1.5)	138.6 C
7α	1.68 dddd (14.0, 14.0, 5.0, 4.5)	17.1 CH ₂	17		172.6 C
7β	2.17 m		18		175.7 C
8	2.35br d (4.5)	41.2 CH	19 _{pro-S}	4.00 d (9.0, 2.0)	76.3 CH ₂
9		36.6 C	19_{pro-R}	4.48 d (9.0)	
			20	1.26 s	31.7

Table S1. ¹H and ¹³C NMR Data of Compound 10 (500/125 MHz, CDCl₃).