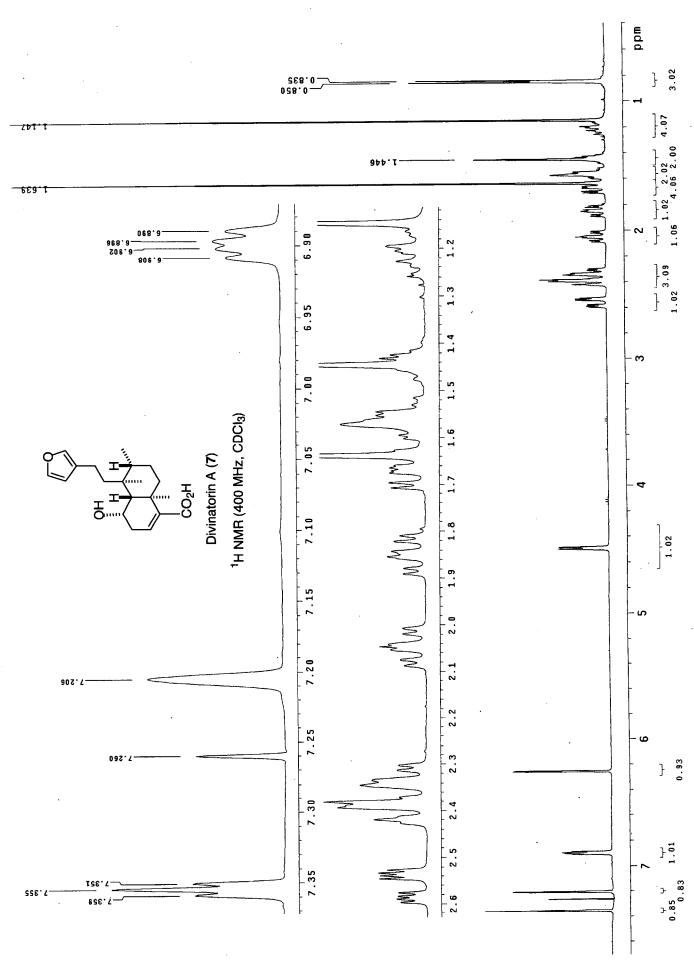
Divinatorins A-C, New Neoclerodane Diterpenoids from the Controlled Sage *Salvia divinorum*.

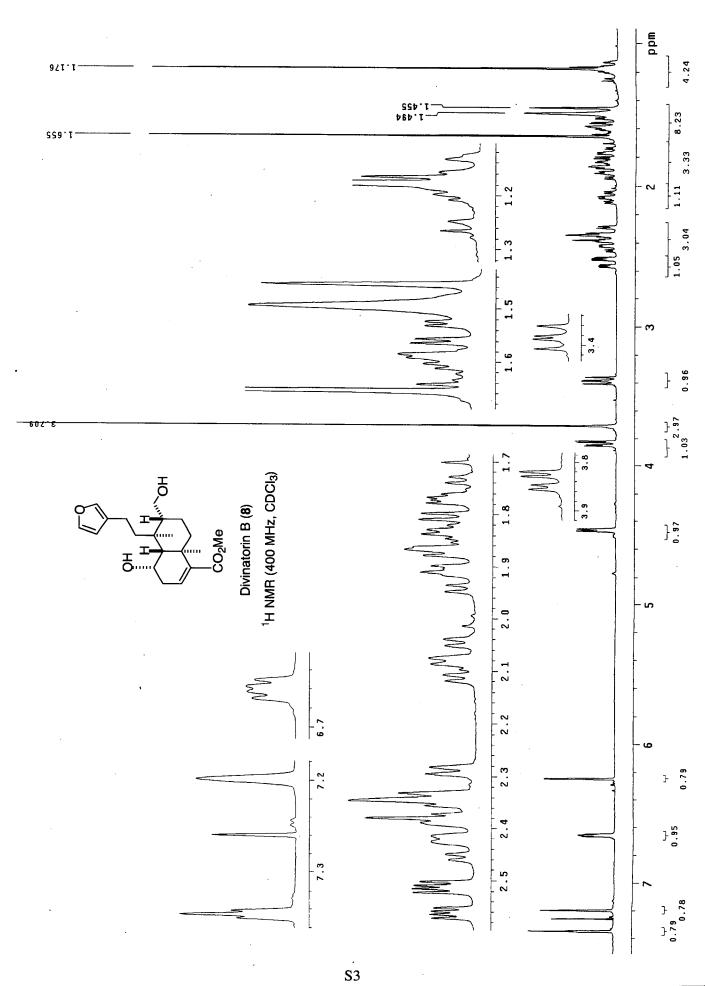
Andrea K. Bigham, Thomas A. Munro, Mark A. Rizzacasa and Roy M. Robins-Brown

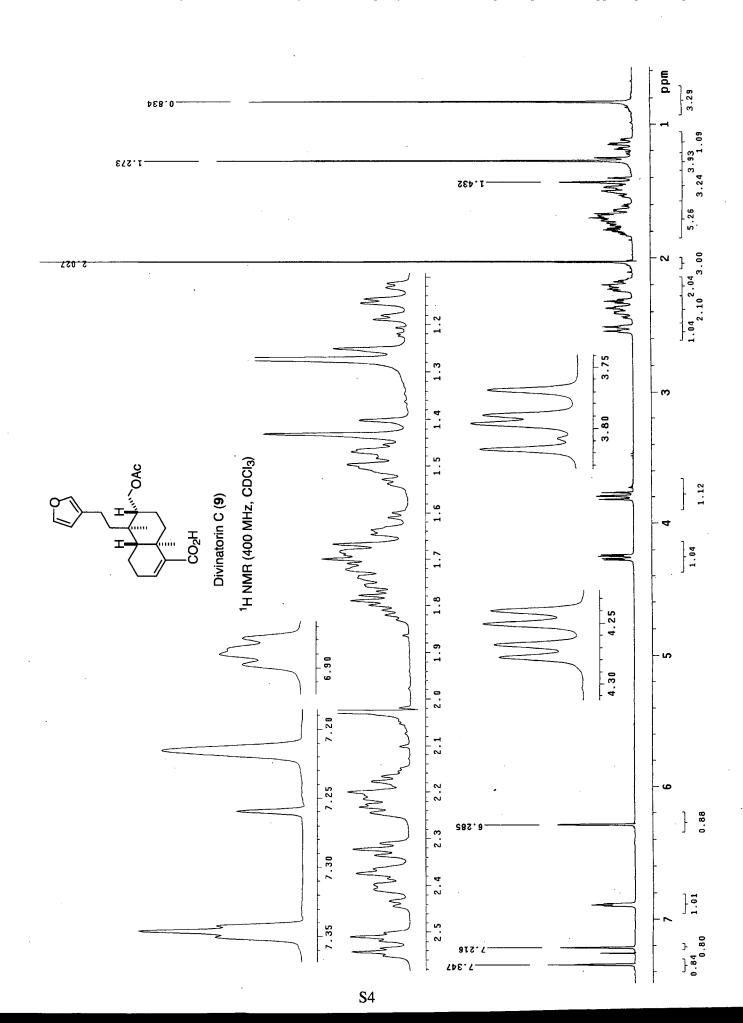
Supporting Information

Table of Contents

¹ H NMR Spectra: Divinatorin A (7)	
Divinatorin B (8)	S 3
Divinatorin C (9)	S 4
¹³ C NMR Spectra: Divinatorins A-C (7-9)	
TLC data (1-14)	S 6
Isolation of (+)-hardwickiic acid (ent-10)	S 7







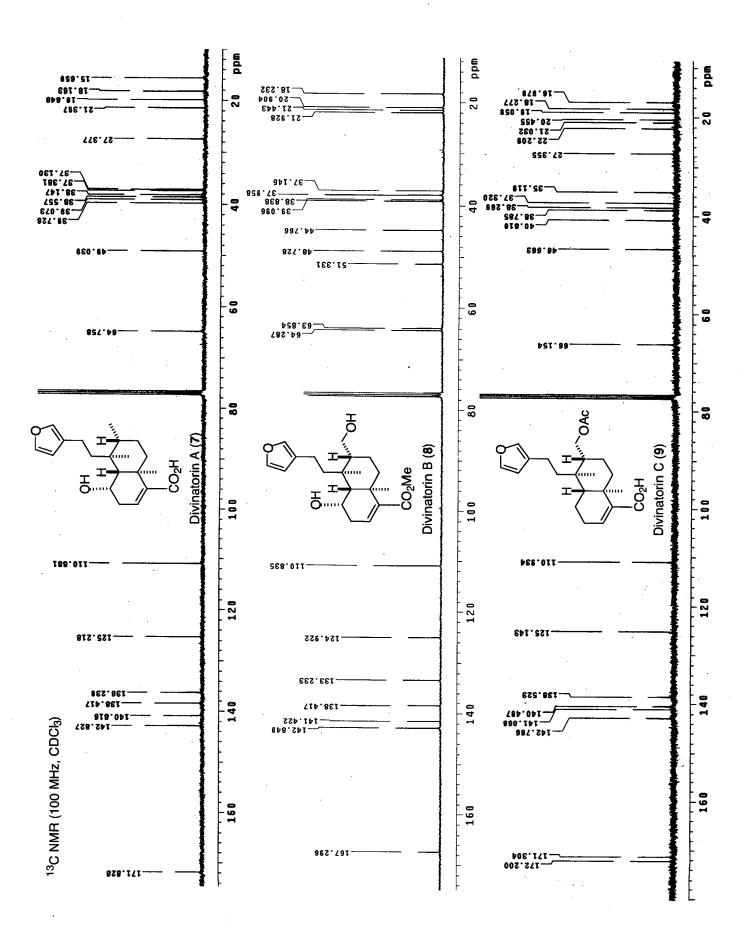


Table S1. TLC data for compounds 1-14 (hR_f on silica gel).

		<u></u> -
	70% Et ₂ O/petrol	10% acetone/CH ₂ Cl ₂
Salvinorin A (1)	24	57
B (2)	14	37
C (3)	31	60
D (4)	18	25
E (5)	23	47
F (6)	24	40.
Divinatorin A (7)	37	15
B (8)	31	31
C (9)	50	39
Hardwickiic acid (10)	. 64	45
Oleanolic acid (11)	66	65
Presqualene Alcohol (12)	44	34
Peplusol (13)	. 75	73
(E)-Phytol (14)	59	58

Isolation of (+)-hardwickiic acid (ent-10): The methyl ester (ent-10b) was isolated from copaiba balsam following the procedure of Costa et al,¹ employing CH_2N_2 in Et_2O for the methylation step. Hydrolysis proved challenging (refluxing in KOH/MeOH gave only slow decomposition); we therefore employed the procedure of Kabalka et al.² The ester ent-10b (32 mg, 97 μ mol) was dissolved in acetone. KF/Al₂O₃ (220 mg, 40% w/w KF) was added and the acetone evaporated under reduced pressure. This was irradiated in a microwave oven (650 W output) at 100% power for 8 minutes, then cooled. Minimal water was added and stirred for 5 minutes, then filtered. The filter cake was rinsed with water (× 2). The filtrate was acidified with 10% HCl and extracted with CHCl₃ (× 4). The pooled organic extracts were dried (MgSO₄) and evaporated to give 14 mg crude product. Flash column chromatography on silica gel (3 g) in 80% Et_2O /petrol gave ent-10 (5 mg, 16 μ mol). Extraction of the alumina filter cake with CHCl₃ (× 3) gave, after drying and evaporation, starting material ent-10b (11 mg).

(+)-hardwickiic acid (ent-10): semicrystalline film; $[\alpha]^{19}_D$ +81° (c 0.155, CHCl₃) [lit.³ for 10: -85.5°]. Other spectroscopic data (¹H and ¹³C NMR, FTIR) matched reported values.³

- 1. Costa, M.; Tanaka, C. M. A.; Imamura, P. M.; Marsaioli, A. J. Phytochemistry 1999, 50, 117-122.
- 2. Kabalka, G. W.; Wang, L.; Pagni, R. M. Green Chem. 2001, 3, 261-262.
- 3. McChesney, J. D.; Clark, A. M.; Silveira, E. R. J. Nat. Prod. 1991, 54, 1625-1633.