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Supplementary Material

The Use of the Toxic Plant *Myoporum montanum* in a Traditional Australian Aboriginal Medicine.

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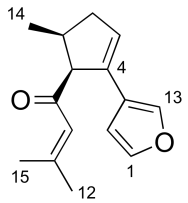
10, 11-Dehydroisomyodesmone (compound 1)

Table 1. NMR spectroscopic data (600 MHz) for compound 1. All data was recorded in $CDCl_3$ and used as reference (δ_H 7.24 ppm for the residual $CHCl_3$ proton; δ_C 77.0 ppm)

Position	δC, type	δH (H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	143.2, CH	7.30 (1H, b*t*, 1.8)	2	3, 13
2	108.3, CH	6.48 (1H, *dd*, 1.8, 0.8)	1, 13	1, 3, 13
3	122.5, *q*C			
4	134.7, *q*C			
5	128.5, CH	6.11 (1H, b*t*, 1.2)	6b*, 8	7
6	40.5, CH_2	2.63 (1H, *ddd*, 2.9, 8.2, 16.6)	6b, 7, 8	4, 5
		2.28 (1H, *ddt*, 1.8, 9.4, 16.6)	6a, 7	4, 5
7	37.8 CH	2.77 (1H, apparent *sept*; 7.6)	6, 8, 14	9
8	64.2, CH	3.60 (1H, *b dd*, 1.5, 9.4)	5, 6a, 7	5, 9
9	202.0, *q*C			
10	123.0, CH	6.07 (1H, *b sept*, 1.2)	12, 15	9, 12, 15
11	155.9, *q*C			
12	27.9, CH_3	1.83 (3H, *d*, 1.2)	10, 15	9, 10, 11, 15
13	139.1, CH	7.22 (1H, *bs*)	2	1, 2
14	15.8, CH_3	1.04 (3H, *d*, 7.3)	7	6, 7, 8
15	20.9, CH_3	2.10 (3H, *d*, 1.2)	10, 12	10, 11, 12

* In the case of a diasterotopic pair of hydrogens: 'a' denotes the downfield proton while 'b' denotes the upfield proton.



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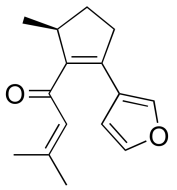

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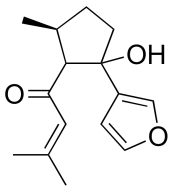

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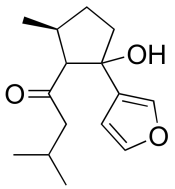

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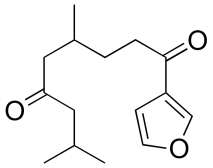

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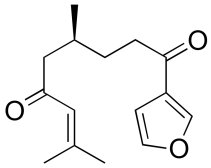


6

10, 11-Dehydromyodesmone (compound 2)

Table 2. NMR (^{1}H 400 MHz; ^{13}C 100 MHz) spectroscopic data for compound 2. All data was recorded in $CDCl_3$ and was use as reference (δ_H 7.24 ppm for the residual $CHCl_3$ proton; δ_C 77.0 ppm).

Position	δ_C, type	δ_H (H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	142.8, CH*	7.32 (1H, *t*, 1.8)	2, 13	2, 3, 13
2	110.6, CH	6.47 (1H, *d*, 1.2)	1	1, 3, 13
3	124.0, *q*C			
4	135.7, *q*C			
5	35.9, CH_2	2.75 (1H, *dddd*, 2.4, 5.2, 7.6, 16.4)	5b, 6	4, 6, 8
		2.63 (1H, *dddd*, 1.6, 6.8, 8.8, 16.4)	5a, 6	4, 6, 8
6	31.3, CH_2	2.17 (1H, *m*)	5, 6b, 7	4, 5, 8
		1.48 (1H, *m*)	5, 6a, 7	5, 7, 14
7	42.9, CH	3.22 (1H, b *sex*, 7.2)	6, 14	4, 8
8	144.1, *q*C			
9	195.2, *q*C			
10	124.8, CH	6.13 (1H, *sept*, 1.2)	12, 15	11, 12, 15
11	154.9, *q*C			
12	28.1, CH_3	1.84 (3H, *d*, 1.2)	10	10, 11, 15
13	142.2, CH*	7.61 (1H, b*s*)	1	1, 2, 3
14	19.8, CH_3	1.09 (3H, *d*, 6.8)	7	6, 7, 8
15	21.2, CH_3	2.17 (3H, *d*, 0.8)	10	10, 11,12

10, 11-Dehydromyoporum ketol (compound 3)

Table 3. NMR (^{1}H: 600 MHz; ^{13}C: 150 MHz) spectroscopic data for compound 3. All data was recorded in $CDCl_3$ and was use as reference (δ_H 7.24 ppm for the residual $CHCl_3$ proton; δ_C 77.0 ppm).

Position	δ_C, type	δ_H (H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	138.8, CH	7.26 (1H, *s*)		
2	109.3, CH	6.22 (1H, *s*)		1, 13
3	130.0, *q*C			
4	81.2, *q*C			
5	42.5, CH_2	2.14 (1H, *m*)	5b, 6b	
		1.96 (1H, *m*)	5a	
6	31.1, CH_2	1.96 (1H, *m*)	6b, 7	
		1.54 (1H, *m*)	5a, 6a, 7	
7	35.7, CH	2.49 (1H, *sept*, 8.0)	6, 8, 14	
8	71.5, CH	2.74 (1H, *d*, 9.0)	7	4, 7, 9, 14
9	200.4, *q*C			
10	125.4, CH	5.99 (1H, b*s*)	12, 15	9, 12, 15
11	156.0, *q*C			12, 15
12	27.6, CH_3	1.77 (3H, *s*)	10	15
13	142.9, CH	7.26 (1H, *s*)		
14	20.7, CH_3	1.07 (3H, *d*, 6.6)	7	6, 7, 8
15	20.6, CH_3	1.91 (3H, *s*)	10	12
OH		2.02 (1H, *s*)		

Myoporum ketol (compound 4)

Table 4. NMR (^{1}H: 400 MHz, ^{13}C: 100 MHz) spectroscopic data for compound 4. All data was recorded in $CDCl_3$ and was use as reference (δ_H 7.24 ppm for the residual $CHCl_3$ proton; δ_C 77.0 ppm).

Position	δ_C, type	δ_H (H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	138.8, CH	7.29 (1H, *s*)	13	2, 3, 13
2	109.3, CH	6.23 (1H, *s*)	13	1, 3, 13
3	130.0, *q*C			
4	81.6, *q*C			
5	43.0, CH_2	2.15 (1H, *m*)	5b, 6	
		1.95 (1H, *m*)	5a, 6	4 and/or 8
6	31.4, CH_2	1.95 (1H, *m*)	6b	4 and/or 8
		1.57 (1H, *m*)	5, 6a, 7	
7	36.2, CH	2.48 (1H, *m*)	6, 8, 14	
8	71.1, CH	2.76 (1H, *d*, 8.4)	7	4, 7, 14
9	217.0, *q*C			
10	53.8, CH_2	2.15 (1H, *m*)	10b	12, 15
		2.03 (1H, *dd*, 7.2, 16.8)	10a	12, 15
11	23.9, CH	1.96 (1H, *m*)	12, 15	
12	22.1, CH_3*	0.66 (3H, *d*, 6.6)	11	10, 11, 15
13	143.1, CH	7.29 (1H, *s*)	1, 2	1, 2, 3
14	20.8, CH_3	1.06 (3H, *d*, 6.6)	7	6, 7, 8
15	22.7, CH_3*	0.80 (3H, *d*, 7.2)	11	10, 11, 12
OH		1.89 (1H, *s*)		

Myoporone (compound 5)

Table 5. NMR (^{1}H: 400 MHz, ^{13}C: 100 MHz) spectroscopic data for compound 5. All data was recorded in $CDCl_3$ and was use as reference (δ_H 7.24 ppm for the residual $CHCl_3$ proton; δ_C 77.0 ppm).

Position	δ ^{13}C, type	δ ^{1}H (no. H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	144.2, CH	7.42 (1H, *t*, 1.7)	2, 13	2, 13
2	108.7, CH	6.74 (1H, *dd*, 0.6, 1.7)	1, 13	1, 13
3	127.0, *q*C			
4	195.0, *q*C			
5	38.2, CH_2	2.73 (2H, *m*)	6	4, 6, 7
6	31.1, CH_2	1.70 (1H, *m*)	5, 6b, 7	5, 7, 8, 14
		1.52, (1H, *m*)	5, 6a, 7	5, 7, 8, 14
7	28.8, CH	2.06 (1H, *sex*, 6.0)	6, 8a, 14	
8	50.6, CH_2	2.37 (1H, 6.0, 16.2)	8b	6, 7, 9, 10, 14
		2.25 (1H, *m*)	8a	6, 7, 9, 10, 14
9	210.0, *q*C			
10	52.4, CH_2	2.24 (2H, *d*, 6.6)	11	9, 11, 12, 15
11	24.5, CH	2.11 (1H, *m*)	10, 12, 15	10
12	22.60*, CH_3	0.886* (3H, *d*, 6.6)	11	10, 11, 15
13	147.1, CH	8.01 (1H, *s*)	1, 2	1, 2, 3
14	19.7, CH_3	0.91 (3H, *d*, 7.2)	7	6, 7, 8
15	22.57*, CH_3	0.890* (3H, *d*, 6.6)	11	10, 11, 12

* assignments may be interchanged

10, 11-Dehydromyoporone (compound 6)

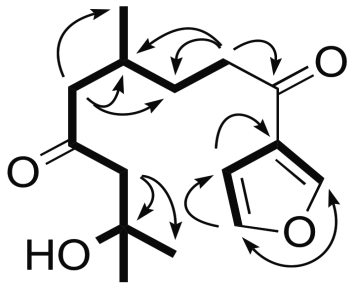
Table 6. NMR (^{1}H: 400 MHz, ^{13}C: 100 MHz) spectroscopic data for compound **6**. All data was recorded in $CDCl_3$ and was use as reference (δ_H 7.24 ppm for the residual $CHCl_3$ proton; δ_C 77.0 ppm).

Position	δ_C, type	δ_H (H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	144.1, CH	7.41 (1H, apparent *t*, 1.6)	2, 13	2, 3, 13
2	108.7, CH	6.74 (1H, *dd*, 0.8, 2.0)	1, 13	1, 3, 13
3	127.6, *q*C			
4	195.1, *q*C			
5	38.2, CH_2	2.73 (2H, *m*)	6	4
6	31.3, CH_2	1.70 (1H, *m*)	5, 7	4, 5, 7, 8, 14
		1.57 (1H, *m*)	5, 7	4, 5, 7, 8, 14
7	29.4, CH	2.06 (1H, apparent *sex*, 6)	6, 8, 14	5, 6, 8, 14
8	51.5, CH_2	2.41 (1H, *dd*, 6.0, 15.6)	7	6, 7, 10, 14
		2.26 (1H, *dd*, 7.6, 15.6)	7	6, 7, 10, 14
9	200.5, *q*C			
10	124.0, CH	6.04 (1H, b *sept*, 1.2)	12, 15	7, 8, 9, 11, 12, 15
11	155.3, *q*C			
12	27.7, CH_3	1.85, (3H, *d*, 0.1.2)	10	10, 11, 15
13	147.1, CH	8.00 (1H, *dd*, 0.8, 1.2)	1, 2	1, 2, 3
14	19.8, CH_3	0.92 (3H, *d*, 6.8)	7	6, 7, 8
15	20.7, CH_3	2.11 (3H, *d*, 0.8)	10	10, 11, 12

11-Hydroxymyoporone (compound 7)

Table 7. NMR (^{1}H: 600 MHz, ^{13}C: 150 MHz) spectroscopic data for compound **7**. All data was recorded in $CDCl_3$ and was use as reference (δH 7.24 ppm for the residual $CHCl_3$ proton; δC 77.0 ppm).

Position	δ ^{13}C, type	δ ^{1}H (no. H, *mult.*, *J* Hz)	^{1}H-^{1}H COSY	HMBC
1	144.2, CH	7.42 (1H, *t*, 1.7)	2, 13	2, 3, 13
2	108.6, CH	6.74 (1H, *dd*, 1.7, 0.6)	1, 13	1, 3, 13
3	127.5, *q*C			
4	194.0, *q*C			
5	37.9, CH_2	2.73 (2H, *m*)	6	4, 6, 7
6	30.9, CH_2	1.72 (1H, *m*)	5, 7	4, 5, 8, 7, 14
		1.57 (1H, *m*)	5, 7	4, 5, 7, 8, 14
7	28.6, CH	2.06 (1H, app. *sextet*, 7.2)	6, 8, 14	6, 14
8	51.6, CH_2	2.42 (1H, *dd*, 6.0, 16.6)	7, 8b, 10	6, 7, 14
		2.28 (1H, *dd*, 7.8, 16.6)	7, 8a, 10	6, 7, 14
9	199.1, *q*C			
10	53.5, CH_2	2.57 (2H, *s*)	8, 15, 12	11, 12, 15
11	69.6, *q*C			
12	29.3, CH_3	1.28 (3H, *s*)	10, OH	10, 11, 15
13	147.0, CH	8.01 (1H, *s*)	1, 2	1, 2, 3
14	19.6, CH_3	0.93 (3H, *d*, 6.6)	7	6, 7, 8
15	29.3, CH_3	1.28 (3H, *s*)	10, OH	10, 11, 12
OH		3.81 (1H, *s*)	12,15	



^{1}H,^{1}H-COSY correlations (**bold** bonds) and significant HMBC correlations (H→C)